SIMULATION STUDY OF DIVIDED WALL DISTILLATION COLUMN

Bachelor inTechnology
In
Chemical Engineering

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CERTIFICATE

Thisistocertifythatthereporttitled,**'Simulation Study of Divided Wall Distillation Column'** submittedby**SaurabhArora(110CH0386)**inpartial fulfillmentof therequirementsfor theawardofBachelor ofTechnology DegreeinChemical EngineeringattheNational Institute OfTechnology,Rourkela isanoriginalworkcarriedoutbyhimunder mysupervisionandguidance.

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ABSTRACT

These days the center is on energy-saving advances. Several techniques have been proposed inorder to improve the efficiency of distillation process; dividing-wall column is one of thesetechniques. Conventionally, distillation columns are connected in series to separatemulti-component mixtures into more than two product streams with high purity prerequisites.

However, in the dividing-wall column, middle section is divided into two sections by inserting avertical wall in the vessel at an appropriate position. Feed is introduced into the pre-fractionatorside of the wall. A side stream is removed from the main column. Therefore, a single dividingwall column can separate a ternary mixture into three pure product streams. The side stream ismostly the intermediate boiling component of the ternary mixture.In the present study a mathematical model of the dividing wall column has been developed,which incorporates the material balance, energy balance, and equilibrium relationships. This model was simulated by taking four columns in an equivalent divided wall distillation column sequence using aspen Plus. This particular design was used to study the separation of three ternary mixtures, Benzene-Toluene-P-Xylene, Benzene-Toluene-O-Xylene and Methanol-Water-Glycerol. The effects of several parameters suchas reflux ratio, number of trays, feed composition, and splitting ratio have been discussed to findthe optimum operating conditions.

Keywords: Aspen Plus, Aspen Simulation, Divided Wall Distillation Column, Steady State Simulation.

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CHAPTER1

INTRODUCTION

INTRODUCTION

Distillation is still the most important thermal separation technology,but in spite of its widespread use and major benefits, a key drawback is its high energy demand generating over 50% of plant operating costs. The last decades led to energy efficient distillation solutions based on process integration and intensification techniques, such as: cyclic distillation, heat-integrated distillation column, reactive distillation, and thermally coupled columns.Dividing-wall column (DWC) – used for ternary separations – is a practical implementation of the Petlyuk configuration, consisting of a pre-fractionator and a main distillation column. A vertical wall is inserted in a DWC at a position such that it splits the column shell into two sections. The feed stream is introduced into the pre-fractionator (feed side of the column) while a side stream is removed from the main column (side stream section). The lightest component goes overhead as distillate and the heaviest component goes out as bottoms, while the side stream contains only the intermediate boiling component. At the top of the wall the refluxed liquid is split between the two sides of the column, while at the bottom the vapor flow is split according to the pressure drop on both sides of the wall. The DWC technology is very appealing to industry as it confers major benefits over conventional distillation: up to 30% reduced investment costs and up to 40% energy savings. Remarkable, these DWC benefits are not limited to ternary separations alone, but they can be present also in azeotropic and extractive distillation, as well as reactive distillation.Dividing wall distillation technology concepts also have a long history. In fact concepts were developed as early as 1933, with the current concept developed in 1946 by Richard Wright. column separates the main column and the side column. In this fully thermally coupled column realised as a DWC the multi-component feed enters the main column, where a cut between low- and high-boiling components takes place. The middle-boiling components of fraction B distribute to the top of the partition wall together with the low boiling components of fraction A (AB) as well as to the bottom of the partition wall, but along with the high-boiling components of fraction C (BC). Thus, as a major advantage of this configuration, the components of fraction C do not enter the side column at the top and the components of fraction A do not enter the side column at the bottom. The mixture of low and middle boiling components (AB) is separated in the upper column section of the main column and the same applies to the high boiling and middle boiling components (BC) which are separated in the lower section of the main column. With regard to the middle boiling components (B) it is obvious, that the composition of B at the top and the bottom of the side column match the composition of B in the main column. There is a peak in the composition of B in the middle of the side column where fraction B is withdrawn. It can be seen that neither low boiling components of fraction A can pass to the bottom part of the side column, nor high boiling

components of fraction C can pass to the upper part of the side column. Thus, contamination of middle boiling fraction B can be avoided.

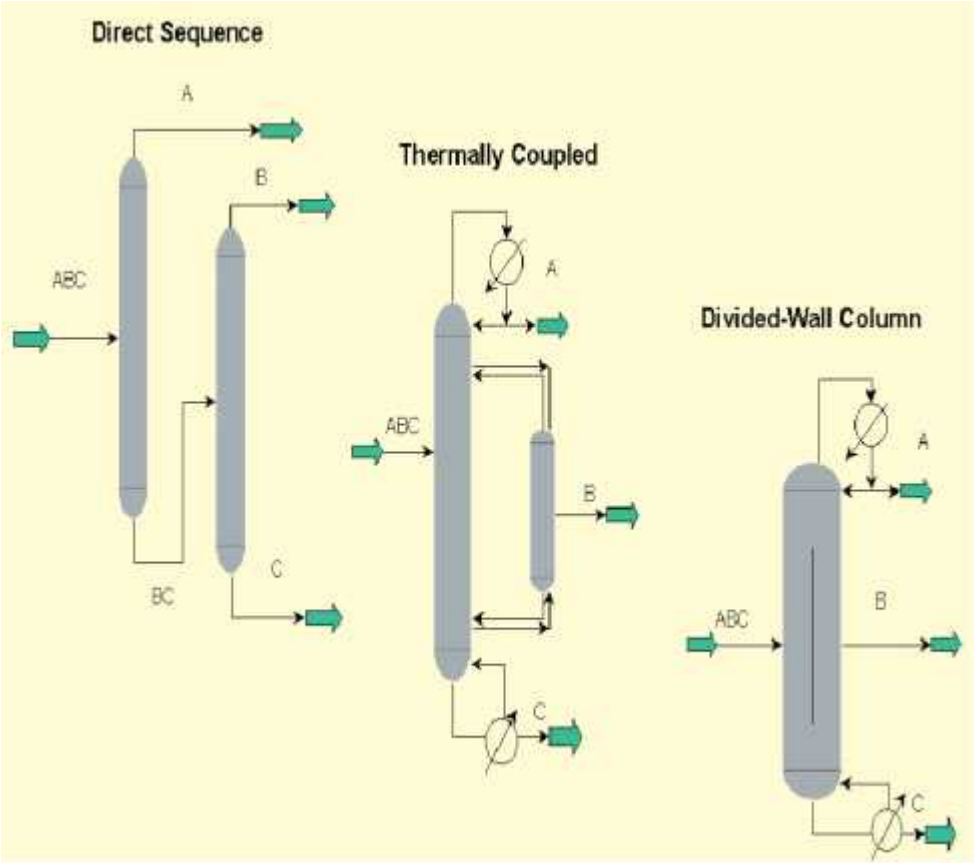


Fig 1: Comparison of various distillation sequences.

CHAPTER 2

LITERATUREREVIEW

LITERATUREREVIEW

For the separation of the three component mixture into pure products, at least a sequence of twosimple distillation columns is needed. Each of these columns has a rectifying and a strippingsection. So the minimum number of column sections is four to receive pure products (Stupin andLockhart, 1972). If one reboiler for each stripping section and one condenser for each rectifyingsection are used, then this leads to the conventional distillation sequences: direct and indirectsplit.
In the separation of the ternary mixtures, dividing wall column (DWC) possesses a significantadvantage in energy saving by avoiding the remixing problem that occurs in a conventionalsequential two-column system. This column also reduces space and investment requirementsover conventional distillation configurations. It is a promising energy–saving alternative forseparating multi-component mixtures (Serra et al., 1999). Due to the wall, which divides thespace in the column, the feed and the side stream –product zones are separated. This wallprevents contamination of the side stream by the feed stream. The dividing wall column hasgreater efficiency than conventional column sequence (Hernadez et al., 2006).The dividing wall column prevents the lateral mixing of liquid and vapour streams in thedistillation column. Heat transfer across the dividing wall can be avoided by thermal insulationof the dividing wall. Especially if very high purities are needed in packed columns, insulation might be useful to suppress undesired wall flow of liquid. Mostly the dividing wall is placed inthe middle, but off-centre positions of the dividing wall are also possible. This might be useful insituations, when the concentration of the medium boiling component is small compared to theoverhead and bottom products (Asprion and Kaibel, 2010).

Van Diggelen et al. (2010) proposed a model of DWC with the assumptions of constant pressure;no vapor flow dynamics, liberalized liquid dynamics, and neglecting energy balance andchanges in enthalpy. They used this model to compare various control strategies. Hiller (2010)developed a nonequilibrium stage model by assuming heat and mass transfer between the liquidand vapor phases for ideal components system. Woinaroschy and Isopescu (2010) used adynamic model for minimizing the distillation start-up time for separation of an ideal benzenetoluene- ethylbenzene ternary mixture and the separation of a non-ideal methanol-ethanol-1-propanol mixture. In this paper, a mathematical model of a dividing wall column has been developed. Several simulation runs of the model have been used to investigate the effects of several parameters and dynamics of the system.
Further Aspen Plus makes it easy to build and run the process simulation model by providing with a comprehensive system of the online process modelling. Process simulation allows one topredict the behaviour of a process by using basic engineering relationships, such as mass andenergy balances, and phase and chemical equilibrium .process simulation enables one to runmany cases, conduct „what if‟ analysis and perform sensitivity analysis and optimisation runs.

With simulation one can design better plants and increase the profitability in the existing plants.Process simulation is helpful throughout the entire life of a process, from research anddevelopment through process design to production.

MathematicalModel

MATHEMATICAL MODEL

The first requirement for our mathematical optimization approach is a model for a distillation column that allows the determination of both structural and operational decisions for all types of column that appears in the various configurations of Figure 1.These include a standardmultifeed two- product column, theprefractionator, andthemain column inthe Petlyuk configuration, and the main column and the sidestream rectifier and stripper in configurations c and d, respectively.

Structural decisions include the number of trays, the position of any feed streams and sideproducts, and alsothe existence or otherwise of a condenser and a reboiler. On the other hand, operational decisions include the reflux ratio in the condenser (if the latter exists), the rate ofheat input tothe reboiler (alsoifthe latter exists), and the flow rates of the various sidestreams. The latter may include both a side product stream and streams connecting the column being modeled to others inthe overall column sequence.

Model Constraints. Theequations and other constraints describing ourcolumn superstructure are presented below.Thevarious symbols used are listed and defined inthe Notation section at the endof the paper. However, it maybe useful to point outhere that the column comprises a maximum of Tmax stages, with stage 1 being the reboiler and stage Tmax the condenser. Thereflux is allowed to be returned to anyone of trays Tminto$T$max- 1; this defines the “topsection” of the column, the rest (trays 2 to Tmin - 1) being its “bottom section”.

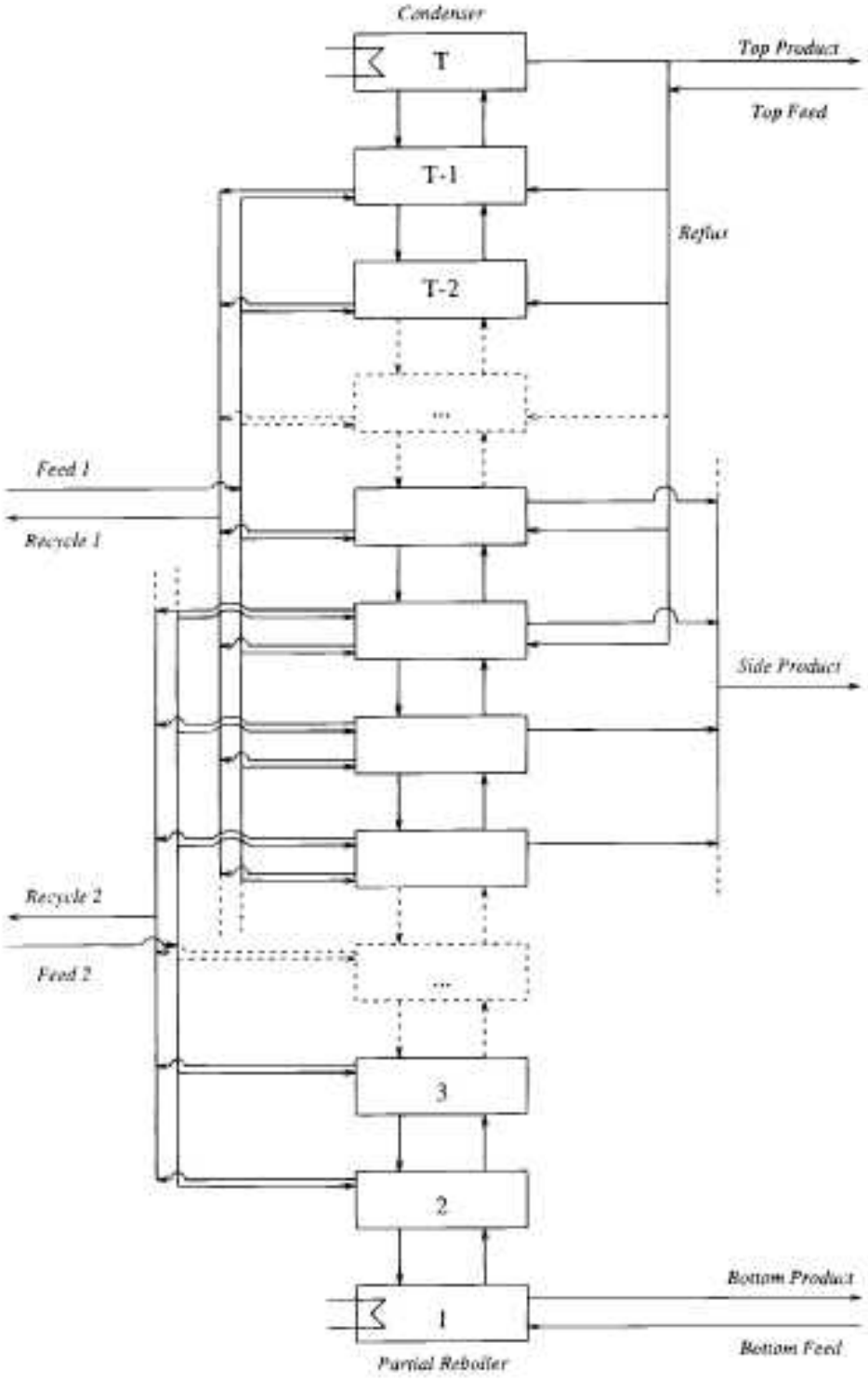


Fig 2: Setup of a continuous Column.

COMPONENT MATERIAL BALANCES

Reboiler

$$L_2 x_{2,c} + F^{\text{bot}} x_c^{F^{\text{bot}}} = P^{\text{bot}} x_c^{P^{\text{bot}}} + V_1 y_{1,c} \qquad \forall\, c \in \{1 \ldots C\} \quad (1)$$

Bottom Section

$$L_{t+1} x_{t+1,c} + V_{t-1} y_{t-1,c} + \sum_{i \in N_{\text{feed}}} f_{t,i} F_i x_{i,c}^F = L_t x_{t,c} + V_t y_{t,c} + \sum_{i \in N_{\text{feed}}} f_{t,i} F_i^{\text{outlet}} x_{i,c}^{F^{\text{outlet}}} + s_t S x_c^S \qquad \forall\, c \in \{1 \ldots C\},\ t \in \{2 \ldots T_{\min} - 1\} \quad (2)$$

Top Section

$$L_{t+1} x_{t+1,c} + V_{t-1} y_{t-1,c} + \sum_{i \in N_{\text{feed}}} f_{t,i} F_i x_{i,c}^F + r_t (R x_{T_{\max},c} F^{\text{top}} x_c^{F^{\text{top}}}) = L_t x_{t,c} + V_t y_{t,c} + \sum_{i \in N_{\text{feed}}} f_{t,i} F_i^{\text{outlet}} x_{i,c}^{F^{\text{outlet}}} + s_t S x_c^S \qquad \forall\, c \in \{1 \ldots C\},\ t \in \{T_{\min} \ldots T_{\max} - 1\} \quad (3)$$

Condenser

$$V_{T_{\max}-1} y_{T_{\max}-1,c} = P^{\text{top}} x_c^{P^{\text{top}}} + R x_{T_{\max},c} \qquad \forall\, c \in \{1 \ldots C\} \quad (4)$$

ENERGY BALANCES

Reboiler

$$L_2 h_2^{\text{liq}} + F^{\text{bot}} h^{F^{\text{bot}}} + Q_{\text{reb}} = P^{\text{bot}} h^{P^{\text{bot}}} + V_1 h_1^{\text{vap}} \quad (5)$$

Bottom Section

$$L_{t+1} h_{t+1}^{\text{liq}} + V_{t-1} h_{t-1}^{\text{vap}} + \sum_{i \in N_{\text{feed}}} f_{t,i} F_i h_i^{\text{F}} = L_t h_t^{\text{liq}} + V_t h_t^{\text{vap}} + \sum_{i \in N_{\text{feed}}} f_{t,i} F_i^{\text{outlet}} h_i^{F^{\text{outlet}}} + s_t S h^{\text{S}}$$

$$\forall t \in \{2 \ldots T_{\min} - 1\} \quad (6)$$

Top Section

$$L_{t+1} h_{t+1}^{\text{liq}} + V_{t-1} h_{t-1}^{\text{vap}} + \sum_{i \in N_{\text{feed}}} f_{t,i} F_i h_i^{\text{F}} + r_t (R h_{T_{\max}}^{\text{liq}} + F^{\text{top}} h^{F^{\text{top}}}) = L_t h_t^{\text{liq}} + V_t h_t^{\text{vap}} + \sum_{i \in N_{\text{feed}}} f_{t,i} F_i^{\text{outlet}} h_i^{F^{\text{outlet}}} + s_t S h^{\text{S}}$$

$$\forall t \in \{T_{\min} \ldots T_{\max} - 1\} \quad (7)$$

Condenser

$$V_{T_{\max}-1} h_{T_{\max}-1}^{\text{vap}} = P^{\text{top}} h^{P^{\text{top}}} + R h_{T_{\max}}^{\text{liq}} + Q_{\text{con}} \quad (8)$$

VAPOR FRACTION DEFINITIONS

Top Product

$$f_{\text{vap}}^{\text{Prod}} = \frac{h^{\text{Prod}} - h_T^{\text{liq}}}{h_{T_{\max}}^{\text{vap}} - h_{T_{\max}}^{\text{liq}}}$$

Product streams taken from feed trays

$$f_{\text{vap},i}^{\text{F}} = \frac{h_i^{\text{Feedin}} - \sum_{t=1}^{T_{\max}} f_{t,i} h_t^{\text{liq}}}{\sum_{t=1}^{T_{\max}} f_{t,i}(h_t^{\text{vap}} - h_t^{\text{liq}})} \qquad \forall\, i \in \{1 \ldots N_{\text{feed}}\} \tag{11}$$

Side Product Streams

$$f_{\text{vap}}^{\text{S}} = \frac{h^{\text{S}} - \sum_{t=1}^{T_{\max}} s_t h_t^{\text{liq}}}{\sum_{t=1}^{T_{\max}} s_t(h_t^{\text{vap}} - h_t^{\text{liq}})}$$

NOTATION

F_i – molar flow of feed i.

h_i – specific enthalpy of feed i.

$x_{i,c}$ - mole fraction of component c in feed i.

P_{top} - molar flow of the top product.

$h^{P\text{top}}$ – specific enthalpy of the top product.

x_C – mole fraction of component c in the top product.

P^{bot} -- molar flow of the bottom product.

$h^{P\text{bot}}$ -- specific enthalpy of the bottom product.

x_c -- mole fraction of component c in the bottom product.

$x_c^{\,s}$ -mole fraction of component c in side product.

h^{S} -specific enthalpy of the side product.

s_t - fraction of S taken from tray t.

R - reflux molar flow rate.

Fi - molar flow rate of the outlet stream at the location of feed i.

$x^{F\text{outlet}}_{\text{i,c}}$ - mole fraction of component c in the outlet stream at location of feed i.

$h_i^{Foutlet}$ - specific enthalpy of the outlet stream at the location of feed i.

F^{bot} - molar flow rate of feed toreboiler.

$x_c^{F\text{bot}}$ - mole fraction of component c in the reboiler feed.

$x_{t,c}$ - liquid-phase mole fraction of component c on tray t .

$y_{t,c}$ - vapor phase mole fraction of component c on tray t .

$\text{h}_\text{t}^{\text{liq}}$ - specific liquid enthalpy on tray t.

L_t - liquid molar flow rate leaving tray t.

V_t - vapor molar flow rate leaving tray t.

T_t -temperature on tray t .

p_t - pressure on tray t.

$f_{t,i}$ - fraction of feed i to tray t.

r_t - fraction of reflux returned to tray t.

CHAPTER 3

SIMULATIONOF TERNARY LIQUID MIXTURE USING DIVIDED WALL DISTILATION COUMN

The software used is Aspen Tech's ASPEN PLUS^{TM}, it allows you to create your own process model, starting with the flowsheet, then specifying the chemical components and operating conditions. ASPEN PLUS^{TM} will take all of your specifications and, with a click of the mouse button, **simulate the model**. The process simulation is the action that executes all necessary calculations needed to solve the outcome of the system, hence predicting its behavior. When the calculations are complete, ASPEN PLUS^{TM} lists the results, stream by stream and unit by unit, so you can observe what happened to the chemical species of your process model.

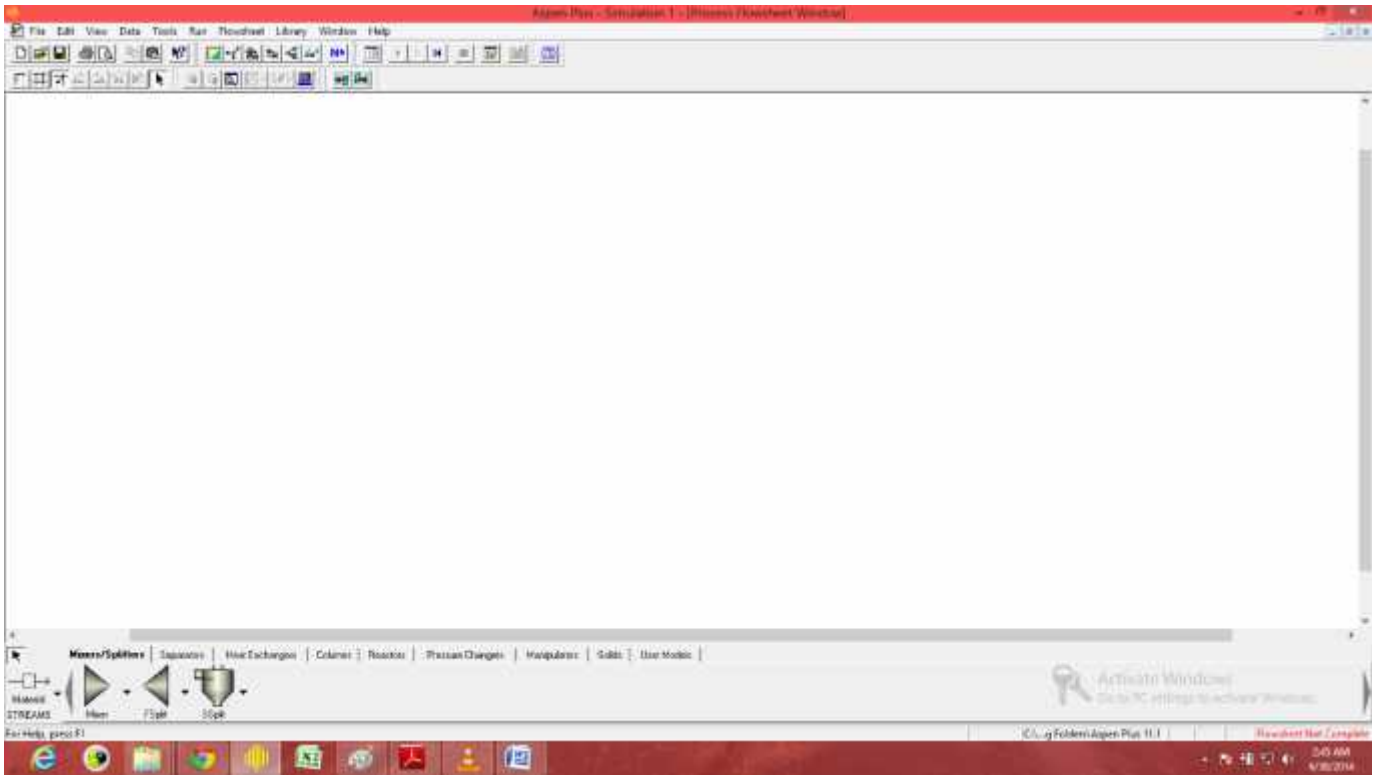


Fig. 3: Aspen Plus Normal Window.

DISTILLATION COLUMN MODEL USED

The columns used for distillation were all **RADFRAC MODELS.** It's a model in which we can To set up an absorber with no condenser or reboiler, set condenser and reboiler to none

on the RadFrac Setup Configuration sheet Either Vaporization or Murphree efficiency on either a stage or component basis can be specified on the RadFrac Efficiency form Tray and packed column design and rating is possible. A second liquid phase may be modeled if the user selects Vapor-Liquid-Liquid as Valid phase. Reboiler and condenser heat curves can be generated.

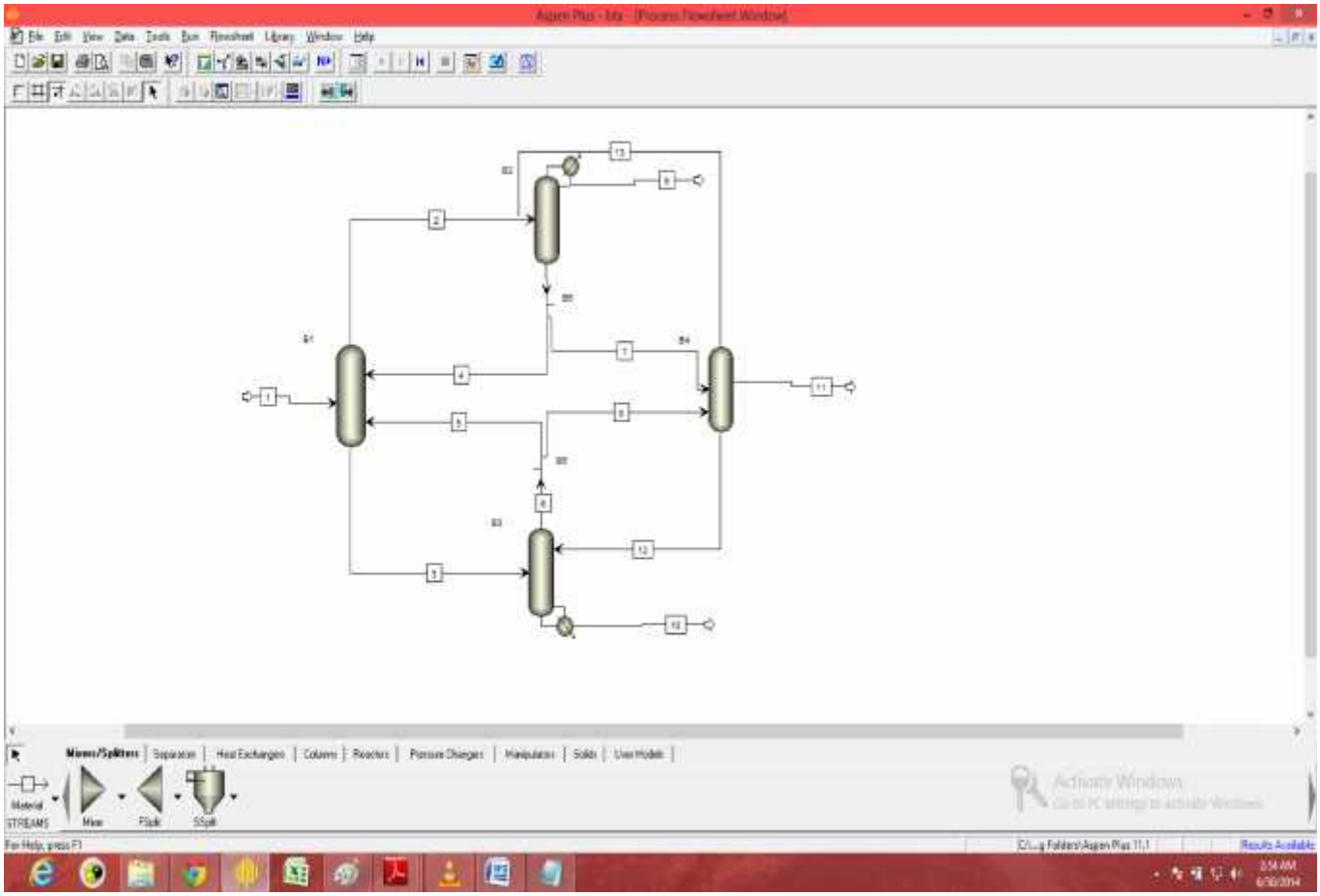


FIG. 4: WORKING MODEL OF A DIVIDED WALL DISTILLATION COLUMN.

The thermodynamic models used for the simulation are namely two.

1. WILSON WITH IDEAL GAS AND HENRY'S LAWS.
2. UNIQAC(Universal Quasi Chemical) MODEL.

UNIQUAC (Universal Quasi Chemical) is an activity coefficient model used in description of phase equilibria [Abrams Prausnitz 1975]. The model is a so-called lattice model and has been derived from a first order approximation of interacting molecule surfaces in statistical thermodynamics. The model is however not fully thermodynamically consistent due to its

two liquid mixture approach. In this approach the local concentration around one central molecule is assumed to be independent from the local composition around another type of molecule.

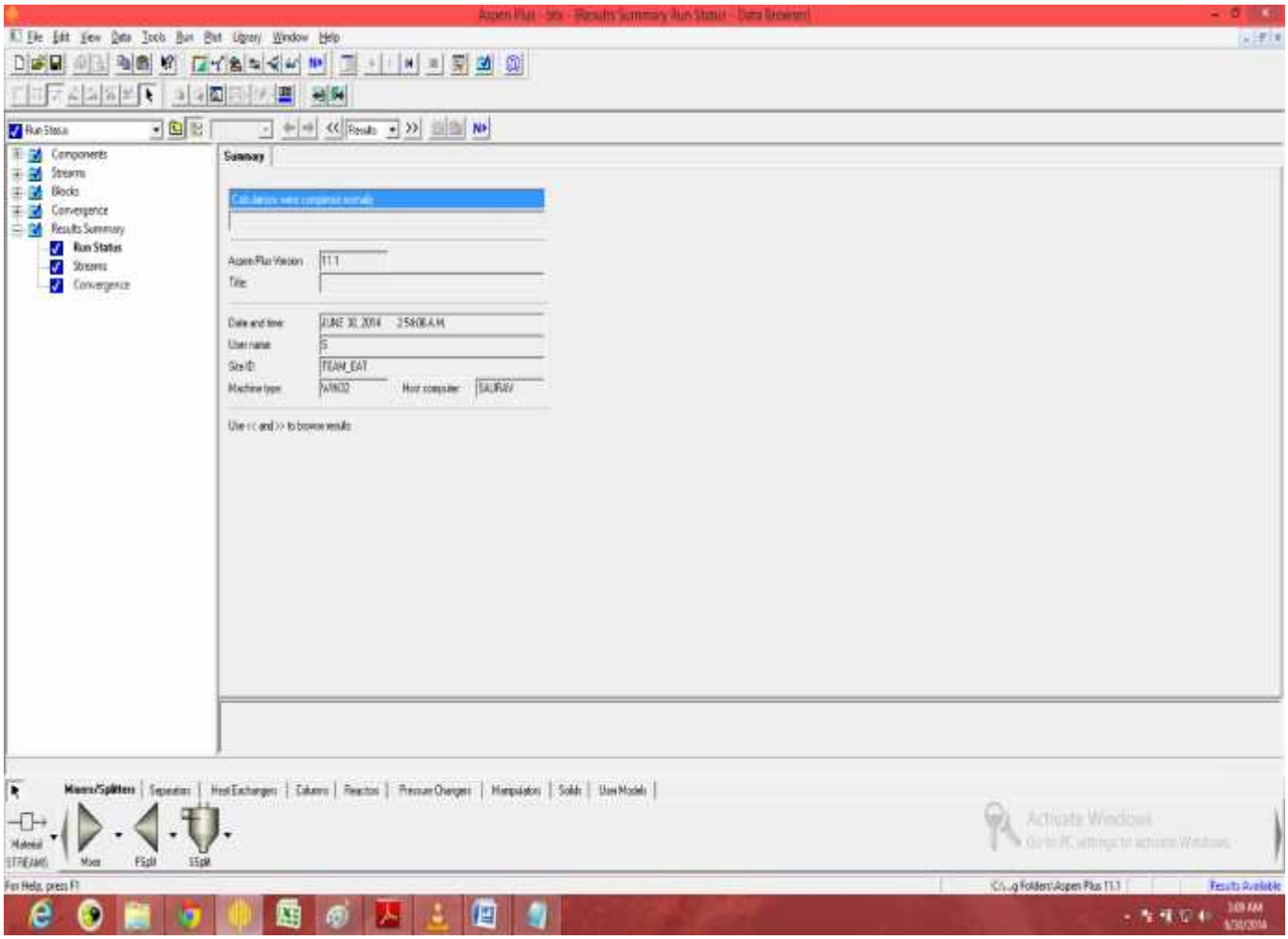


Fig 5: Successful Status of Simulation Run.

This chapter deals with simulation of three ternary mixture systems namely,

1.Benzene-P-Xylene-Toluene.

2.Benzene-O-Xylene-Toluene.

3.Methanol-Glycerol-Water.

This following section dwells into the details of three aforementioned models.

3.1 SIMULATION OF SEPARATION OF A TERNARY MIXTURE OF BENZENE P-XYLENE AND TOLUENE

DETAILS OF SIMULATION.

Table 3.1: Modelling Details for the separation of ternary mixture of Benzene-Toluene-P-xylene using dividing wall distillation column.

PARAMETERS AND CONDITIONS			VALUE
FEED FLOW RATE			100 KMOL/HR
FEED COMPOSITION	Benzene	Mol Fraction	0.2
	P-xylene		0.6
	Toluene		0.2
Number of trays in Prefractionator (B1)			20
Number of trays in Top Section (B2)			15
Number of trays in Bottom Section (B3)			15
Number of trays in Side Draw (B4)			20
Feed tray Position			10
Side Draw Position			6
Reboiler Duty			1743 kW
Split Ratio	Liquid Split		0.4
	Vapor Split		0.3

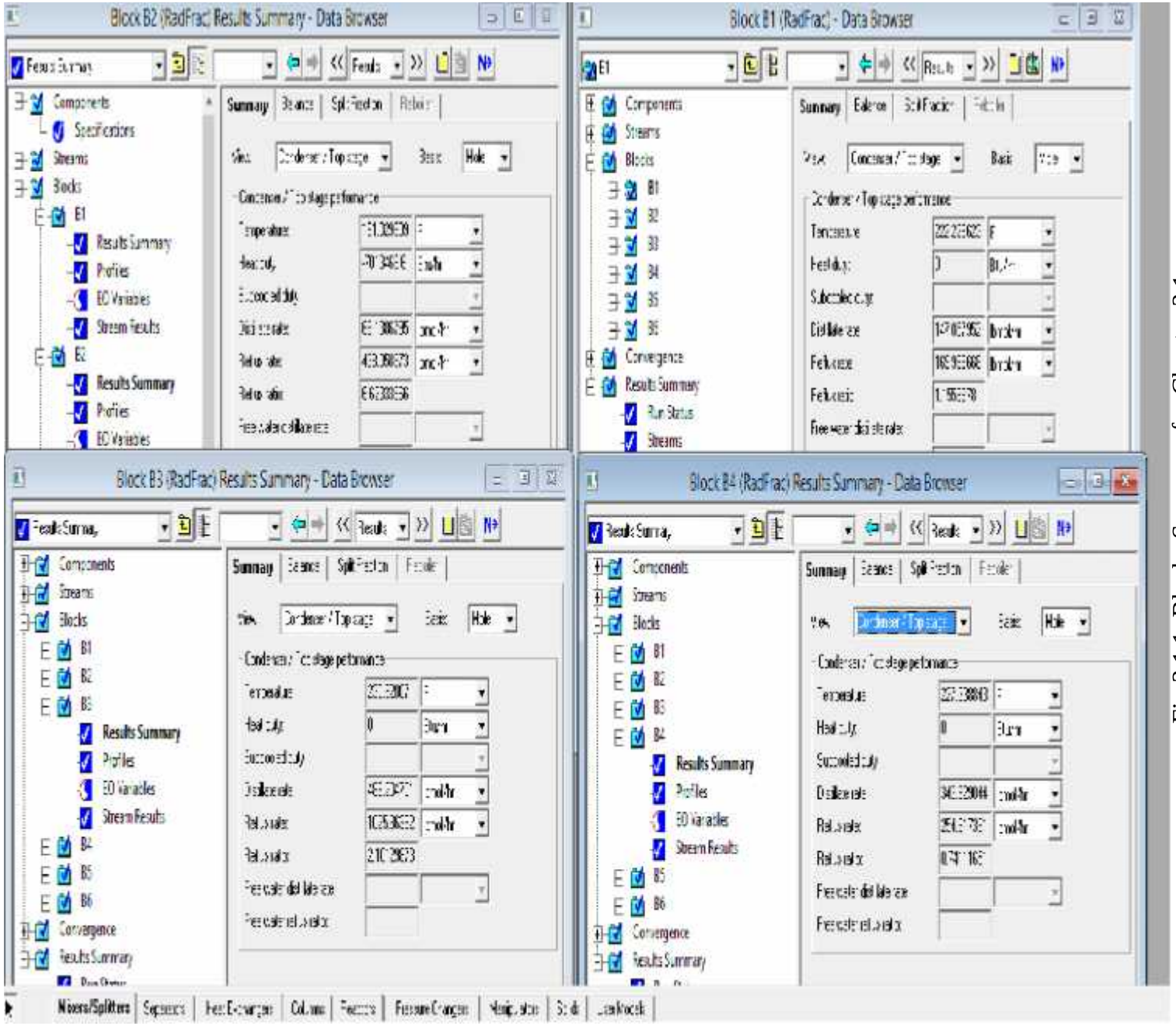


Fig 3.1.1: Blocks Summary for Chapter 3.1

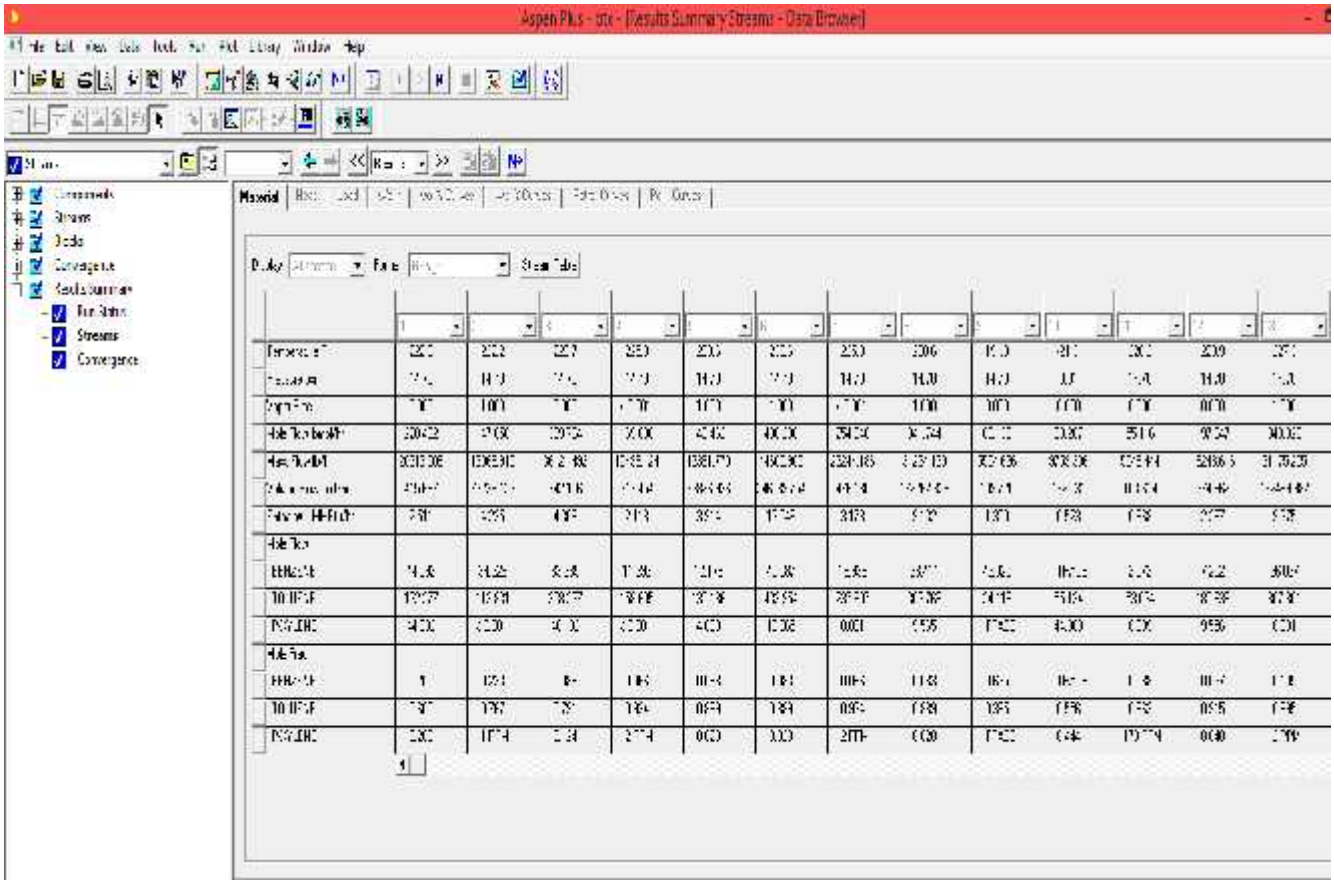


Fig 3.1.2: Results Summary for chapter 3.1.

EFFECT OF REFLUX RATIO ON PRODUCT PURITY AT DISTILLATE

In the dividing wall column, reflux ratio plays an important role. As the reflux ratio is increased, the gradient of operating line for the rectification section moves towards a maximum value of 1. Physically, what this means is that more and more liquid that is rich in the more volatile components are being recycled back into the column.When more overhead liquid product is refluxed in a distillation column the liquid rate in the column increases. Separation then becomes better. While it is seen that increasing the value of reflux ratio increases the purity of top product. It was seen that for a value of RR=12 , the top product was of 99% purity. Whereas the effect of increasing reflux ratio on the purity of bottom product is deteriorating. It was seen that the Product Purity at distillate falls to half from changing the RR from 4 to 10. The effect of RR on Side Stream i.e, Toluene was inconclusive as the purity hardly changed.

	PURITY		
REFLUX RATIO	BENZENE(Top Product)	P-XYLENE(Bottom Product)	TOLUENE(Side Stream)
4	0.44359276	0.62690577	0.96442183
5	0.51765872	0.52461508	0.96355315
6	0.59056487	0.46822269	0.96269543
7	0.66212441	0.43260636	0.96198755
8	0.73220377	0.40812474	0.96141477
10	0.86751463	0.37683161	0.96056408

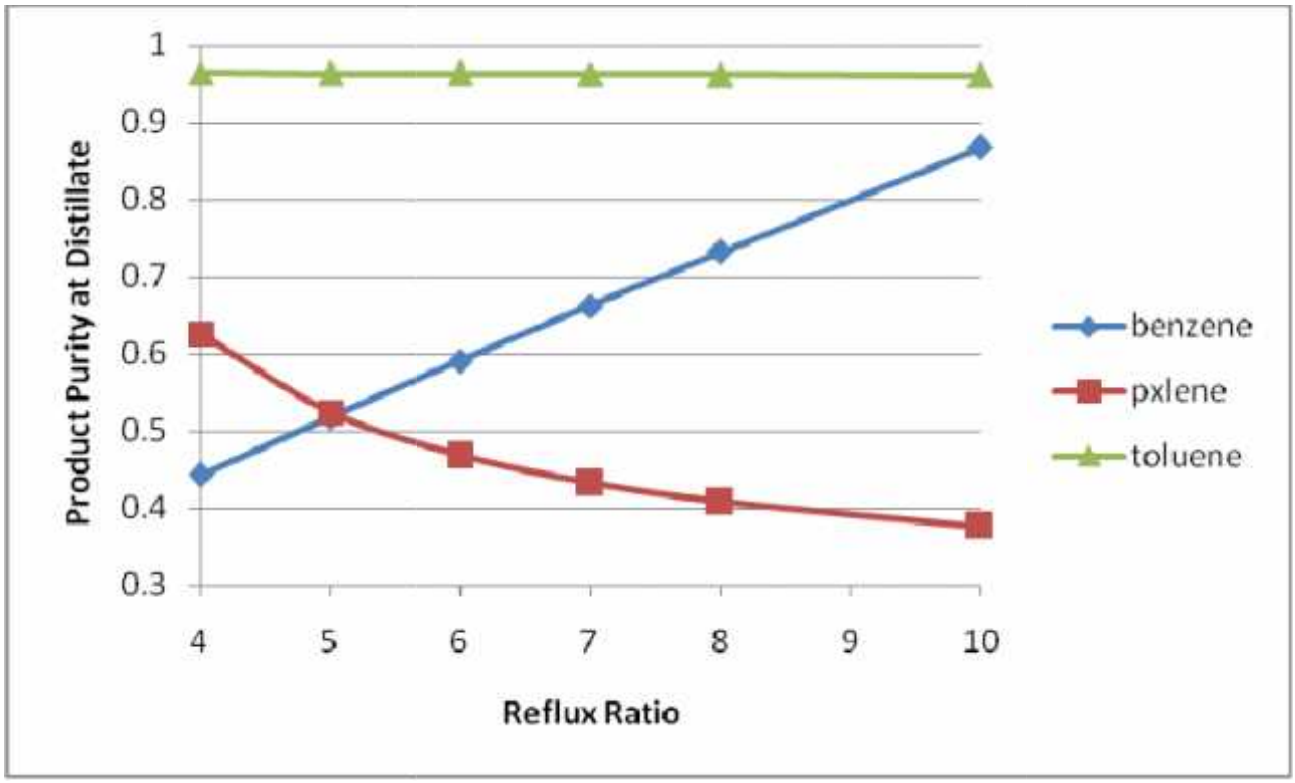


Fig 3.1.3: Graph between Product Purity at distillate v/s Reflux Ratio.

EFFECT OF FEED STAGE ON PRODUCT PURITY AT DISTILLATE

FEED TRAY POSITION	PURITY BENZENE(Top Product)	P-XYLENE(Bottom Product)	TOLUENE(Side Stream)
6	0.63618928	0.4443057	0.96393367
7	0.63625118	0.44435412	0.96331239
8	0.63585425	0.44433675	0.962853
9	0.63556719	0.44435332	0.96250647
10	0.6353375	0.4443457	0.96223681
13	0.63479527	0.44435557	0.96158636

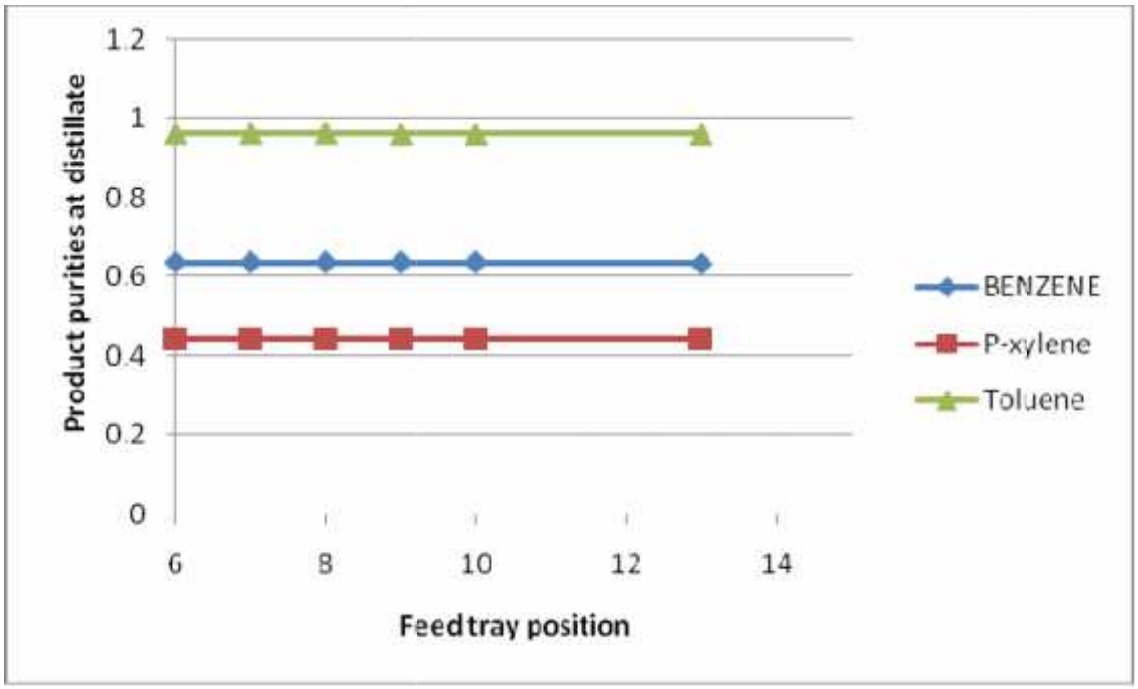
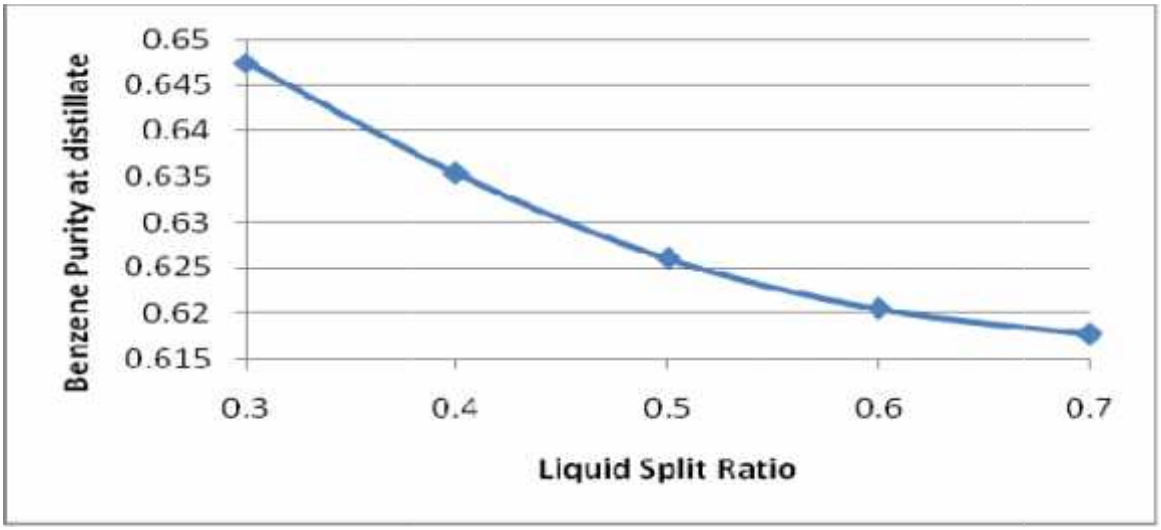


Fig 3.1.4: Graphs between Product Purity at distillate v/s Feed Stage.

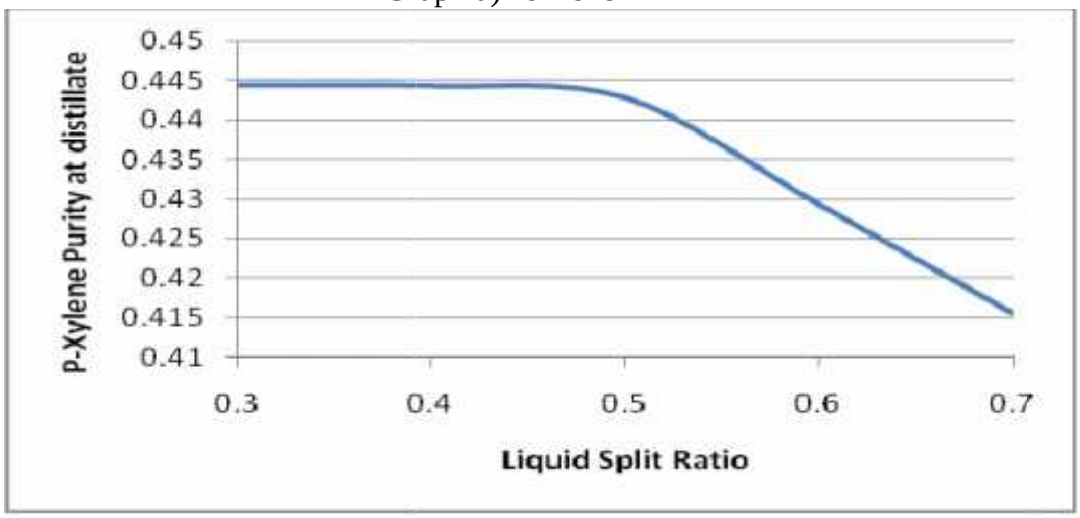
Selection of feed stage is an important factor for Product Purity at distillate. As the feed stage is moved lower down the column, the top composition becomes less rich in the more volatile component while the bottoms contains more of the more volatile component.Generally speaking, if the feed enters in higher tray the light components concentrations in overhead will be increased and in bottom outlet will be decreased. As the feed stage is moved lower down the column, the top composition becomes less rich in the more volatile component while the bottoms contains more of the more volatile component. However, the changes in top composition is not as marked as the bottoms composition.The position of the feed stage has minimal effect on Product Purity at distillate yet as the feed stage in the pre fractionator is lowered the side stream was seen to be unaffected. But purity of both top and bottom product were decreasing with increasing the feed stage. The maximum purity of both of these components were found out to be at the 7^{th} tray (out of a total of 20 trays).

EFFECT OF LIQUID SPLIT FRACTION ON PRODUCT PURITY AT DISTILLATE

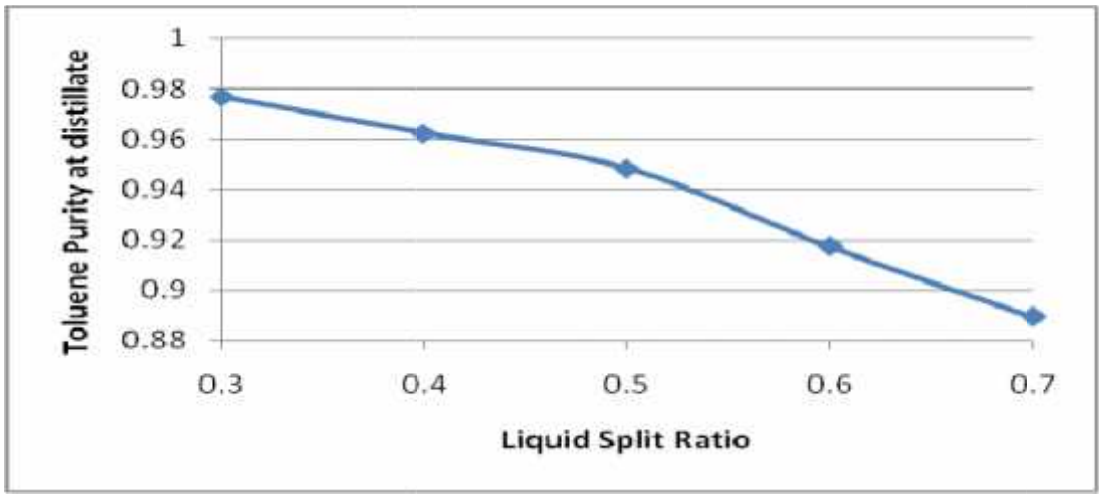
liquid split ratio	benzene(Top Product)	p-xylene(Bottom Product)	toluene(Side Stream)
0.3	0.64743656	0.44444349	0.97690299
0.4	0.63533906	0.44434257	0.96223662
0.5	0.62604943	0.44274973	0.94821757
0.6	0.62051595	0.4292383	0.91723062
0.7	0.61771515	0.41553716	0.88925453



Graph a)Benzene



Graph b)P-xylene



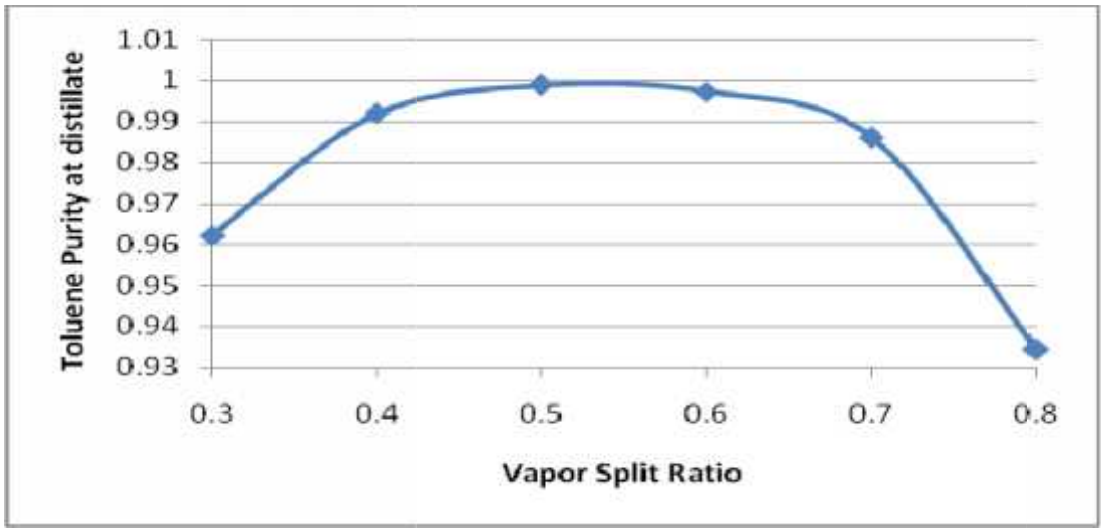
Graph c) Toluene

Fig 3.1.5: Graph between Product Purity at distillate v/s Liquid Split Fraction.

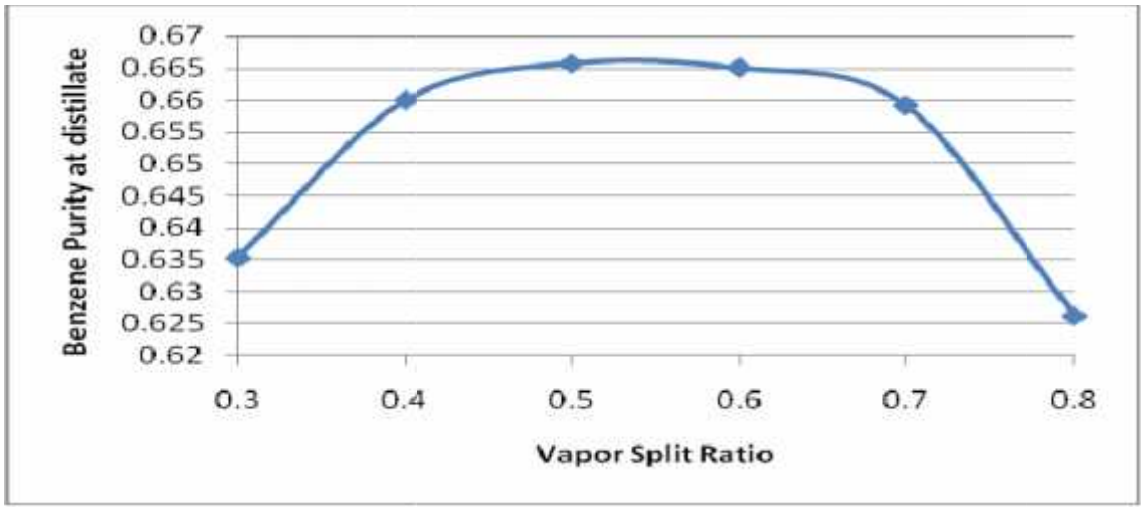
The liquid split factor in the dividing wall column decides how much quantity of the liquid will enter the prefractionator from the rectifying section. As we are supplying the feed in the prefractionator column, the fraction of liquid to be distributed coming from the rectifying section should be less in comparison with the main column to maintain the liquid hold up in both sections. Increasing the liquid split ratio from 0.3 to 0.4 the purity of Benzene and Toluene decreases from 64.7% to 63.5% and 97.6% to 96.2%. However P-xylene is rather unaffected.

EFFECT OF VAPOR SPLIT ON PRODUCT PURITY AT DISTILLATE

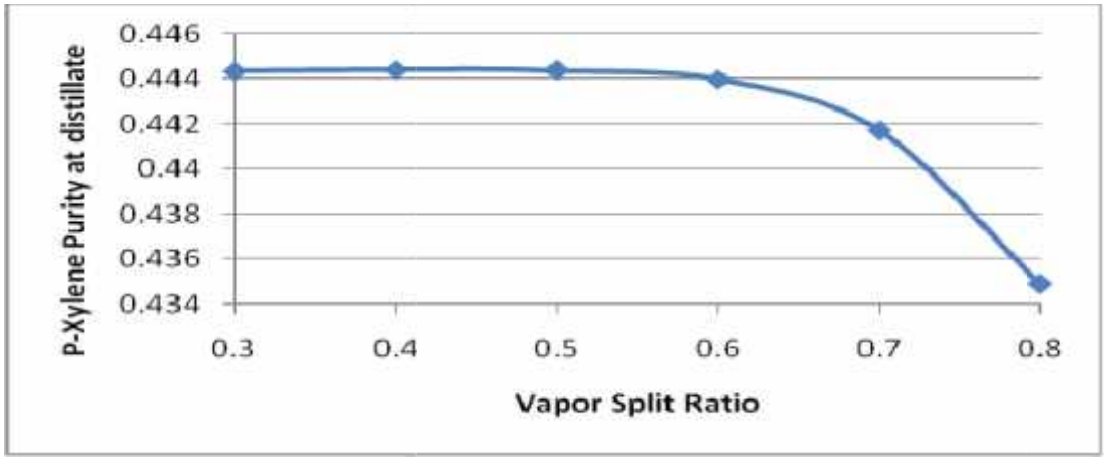
vapor split ratio	benzene(Top Product)	p-xylene(Bottom Product)	toluene(Side Stream)
0.3	0.63533906	0.44435591	0.96223662
0.4	0.65989888	0.44443195	0.99183656
0.5	0.6658075	0.44439564	0.99888582
0.6	0.66505035	0.44400298	0.99725751
0.7	0.65906469	0.44171705	0.98598882
0.8	0.62626815	0.43492385	0.93439086



Graph a)Toluene



Graph b) Benzene



Graph c) P-Xylene

Fig 3.1.6: Graph between Product Purity at distillate v/s Vapor Split Fraction.

The vapour split factor in the dividing wall column decides how much quantity of the vapour will enter in the prefractionator from stripping section. It is seen that when we increase the vapor split from 0.3 to 0.5 the purity of both benzene and toluene gradually increase and attain a maxima, respectively increasing from 96.2% to 99.8% and 63.5% to 66.5%. Then it gradually decreases all along. However, only a change of around 50% in the vapor split ratio slightly transpires any change in the purity f P-Xylene from 44.4% to 43.4%.

EFFECT OF REBOILER DUTY ON PRODUCT PURITY AT DISTILLATE

The amount of energy used is basically depicted by reboiler duty. This simulation has varied the value of reboiler duty from 1650 kW to 2000 kW and the effect on P-xylene purity was not remarkable. However the increase of Reboiler duty from 1650 kW to 2000 kW increased the purity of both Benzene and toluene by approximately 1% each, still proving that Divided Wall Columns are efficient in low energy situation too.

REBOILER DUTY(M.W)	BENZENE(Top Product)	PURITY P-XYLENE(Bottom Product)	TOLUENE(Side Stream)
1.65	0.63413327	0.666426	0.96055856
1.7	0.63550853	0.66646151	0.96226791
1.743	0.63663866	0.66652039	0.96366977
1.85	0.63927809	0.66656639	0.96691386
1.95	0.64152939	0.66661433	0.96966822
2	0.64259322	0.66658745	0.97095604

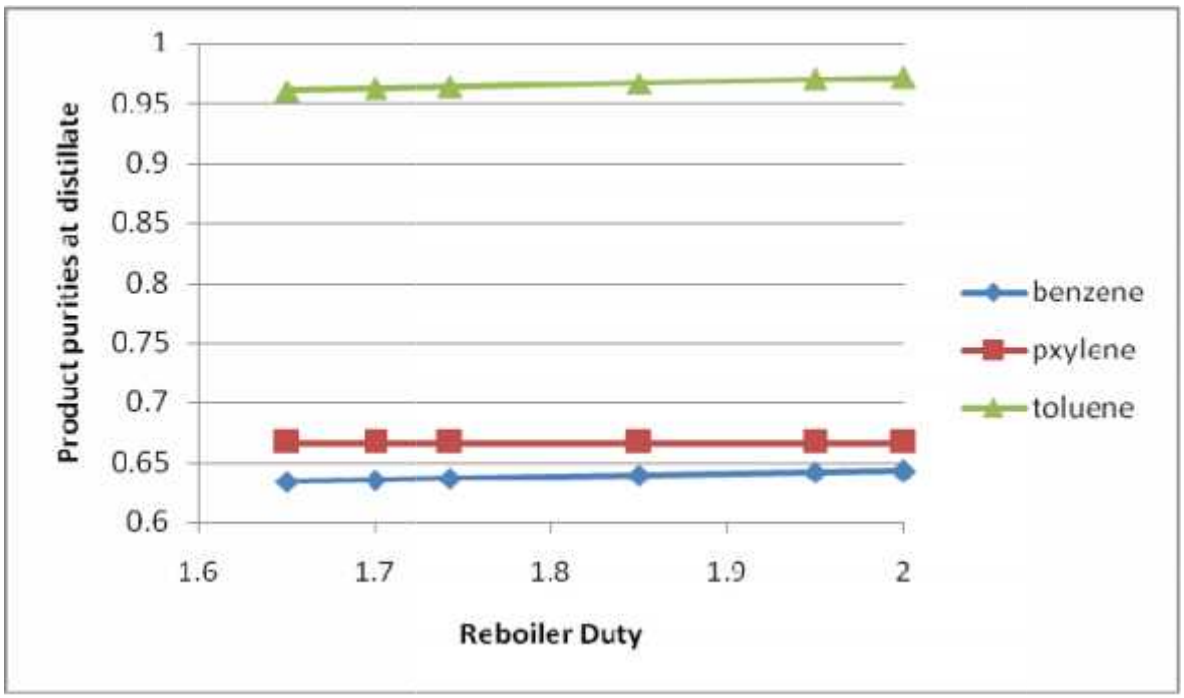


Fig 3.1.7: Graph between Product Purity at distillate v/s Reboiler Duty.

3.2SIMULATION OF SEPARATION OF A TERNARY MIXTURE OF BENZENE O-XYLENE AND TOLUENE USING DIVIDING WALL DISTILLATION COLUMN.

DETAILS OF SIMULATION.

Table 3.2:Modelling Details for the separation of ternary mixture of Benzene-Toluene-O-xylene using dividing wall distillation column.

PARAMETERS AND CONDITIONS			VALUE
FEED FLOW RATE			1000mols/s
FEED COMPOSITION	Benzene	Mol Fraction	0.3
	O-xylene		0.4
	Toluene		0.3

Number of trays in Prefractionator (B1)		24
Number of trays in Top Section (B2)		8
Number of trays in Bottom Section (B3)		12
Number of trays in Side Draw (B4)		24
Feed tray Position		12^{th} stage of pre-fractionator
Side Draw Position		11^{th} of main column
Reboiler Duty		40.54 MW
Split Ratio	Liquid Split	0.353
	Vapor Split	0.627

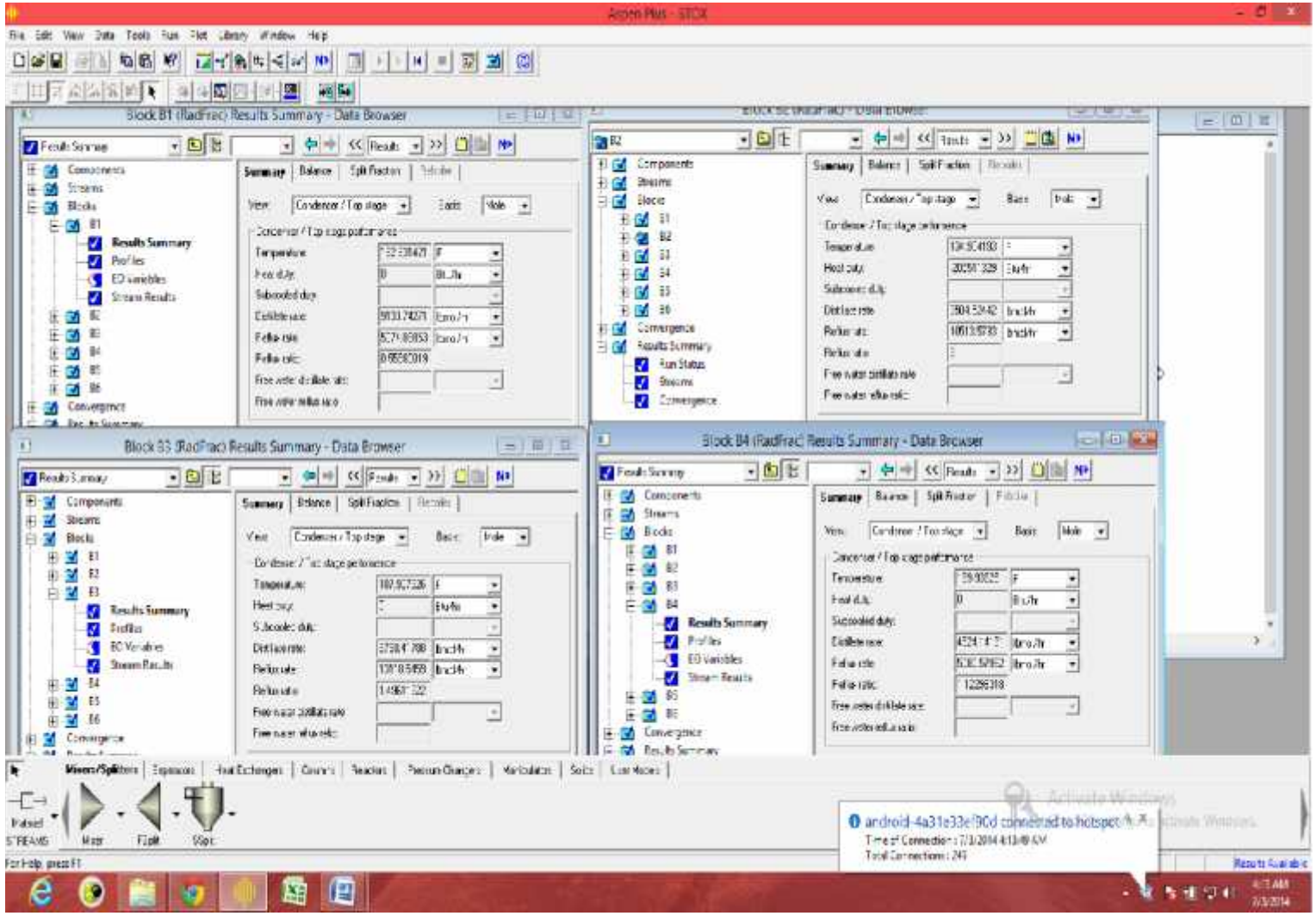


Fig 3.2.1: Blocks Summary for Chapter 3.2.

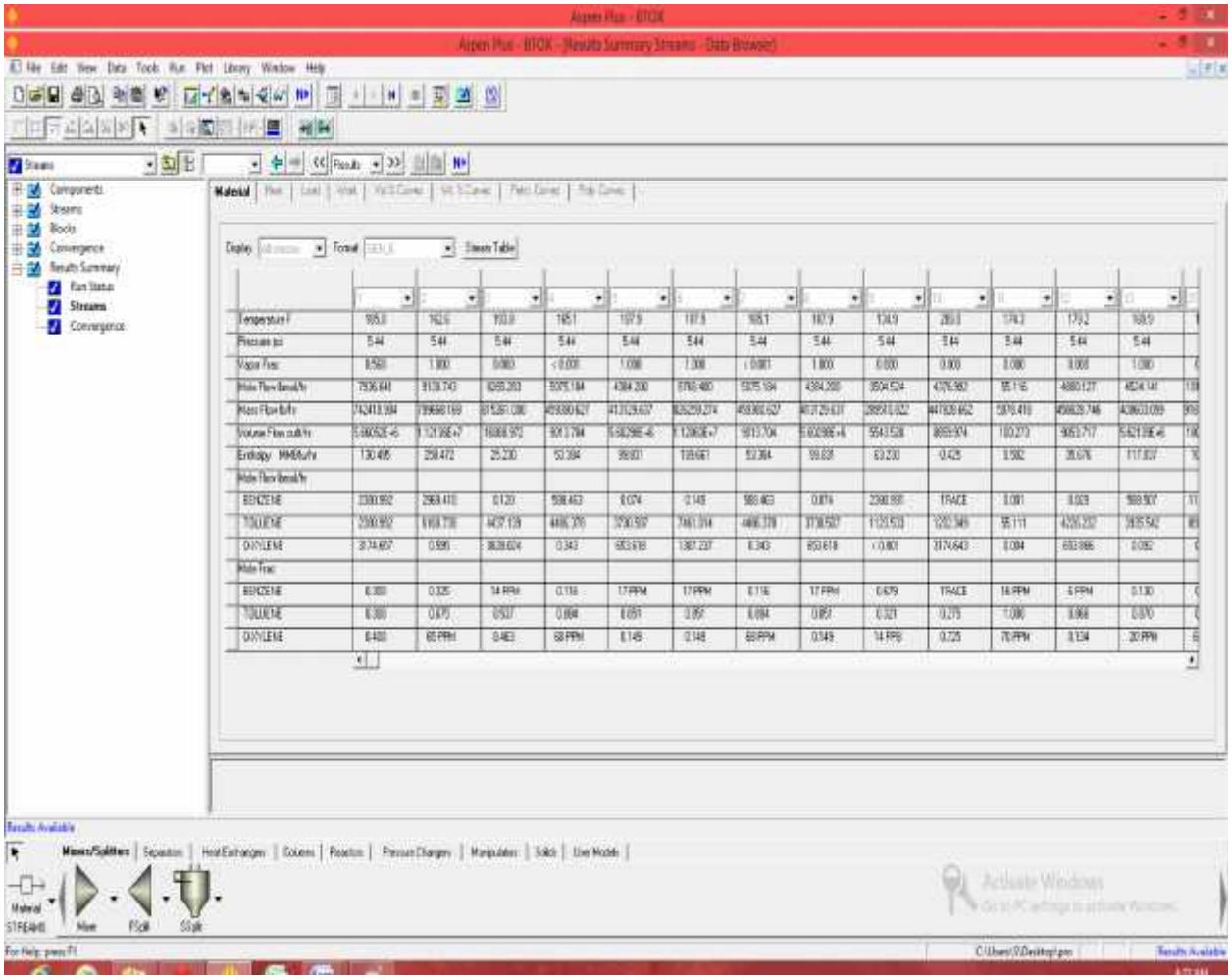


Fig 3.2.2: Results Summary for Chapter 3.2.

EFFECT OF REFLUX RATIO ON PRODUCT PURITY AT DISTILLATE

In the dividing wall column, reflux ratio plays an important role.s the reflux ratio is increased, the gradient of operating line for the rectification section moves towards a maximum value of 1. Physically, what this means is that more and more liquid that is rich in the more volatile components are being recycled back into the column.When more overhead liquid product is refluxed in a distillation column the liquid rate in the column increases. Separation then becomes better.While it is seen that increasing the value of reflux ratio increases the purity of top product. It was seen that the purity of top product i.e , benzene increased greatly as the values of reflux ratio was increased from 2 to 5. The increase was from 52% to 97.4%. The effect of increasing the reflux ratio for the bottom product was deteriorating. Values decreasing from 96%(RR=2) to 58.3% . The purity of Toluene hardly changed over varying reflux ratio.

	PURITY		
REFLUX RATIO	BENZENE(Top Product)	O-XYLENE(Bottom Product)	TOLUENE(Side Stream)
2	0.5205722	0.95972576	0.99745512
3	0.67940499	0.72530247	0.99991408
4	0.83145619	0.63266728	0.99994043
5	0.97432353	0.58380205	0.99990989

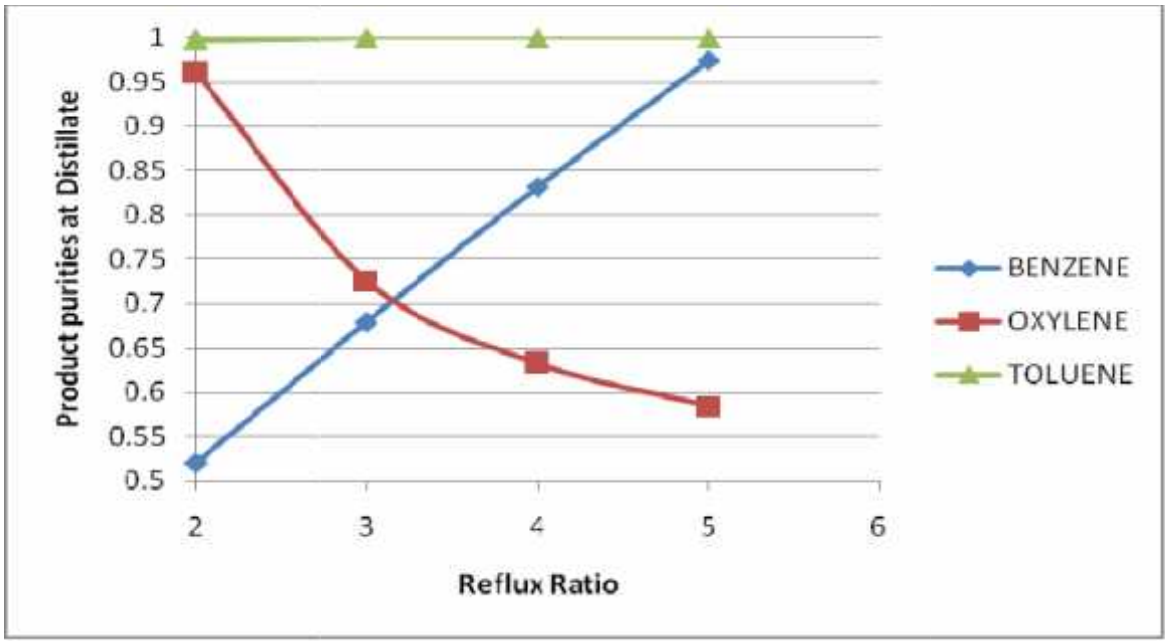


Fig 3.2.3: Graph between Product Purity at distillate v/s Reflux Ratio.

EFFECT OF FEED STAGE ON PRODUCT PURITY AT DISTILLATE

Selection of feed stage is an important factor for Product Purity at distillate. As the feed stage is moved lower down the column, the top composition becomes less rich in the more volatile component while the bottoms contains more of the more volatile component.Generally speaking, if the feed enters in higher tray the light components concentrations in overhead will be increased and in bottom outlet will be decreased. As the feed stage is moved lower down the column, the top composition becomes less rich in the more volatile component while the bottoms contains more of the more volatile component.. However, the changes in top composition are not as marked as the bottoms composition. As the feed stage is moved lower down the column, the top composition becomes less rich in the more volatile component while the bottoms contains more of the more volatile component.

Having said that, the product composition was not seemingly affected in the simulation.

FEED TRAY POSITION	BENZENE(Top Product)	O-XYLENE(Bottom Product)	TOLUENE(Side Stream)

10	0.67940436	0.72529959	0.99962509
11	0.67940463	0.72530377	0.9998276
12	0.67940499	0.72530247	0.99991408
15	0.67940382	0.72530358	0.99993073
24	0.67897871	0.72529926	0.97280243

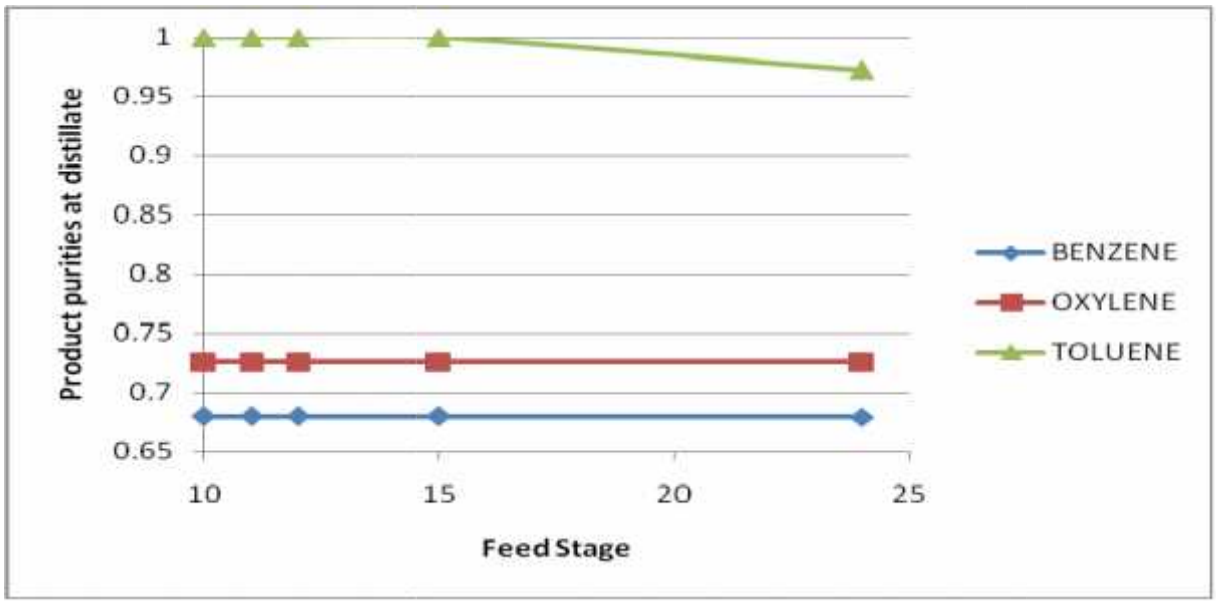


Fig 3.2.4: Graph between Product Purity at distillate v/s Feed Stage.

EFFECT OF LIQUID SPLIT FRACTION ON PRODUCT PURITY AT DISTILLATE

The liquid split factor in the dividing wall column decides how much quantity of the liquid will enter the prefractionator from the rectifying section. As we are supplying the feed in the prefractionator column, the fraction of liquid to be distributed coming from the rectifying section should be less in comparison with the main column to maintain the liquid hold up in both sections. The effect of increasing the liquid split ratio from 0.2 to 0.9 was studied and it was seen that changing the liquid split ratio didn't seem to effect the product purities of Top and Bottom product (Benzene and o-Xylene). The value of side stream purity initially increased with increasing liquid split ratio, achieved a maxima and then started decreasing. The maximum value of Toluene purity (Side Stream) was observed to be at 60% split and was 99.99% pure.

Liquid split ratio	benzene(Top Product)	O-xylene(Bottom Product)	toluene(Side Stream)
0.2	0.67934658	0.72244017	0.77299383

0.3	0.67933508	0.72337635	0.84823167
0.4	0.67938962	0.7246731	0.94935261
0.6	0.67940263	0.72529668	0.9998978
0.9	0.67898764	0.72112169	0.64044296

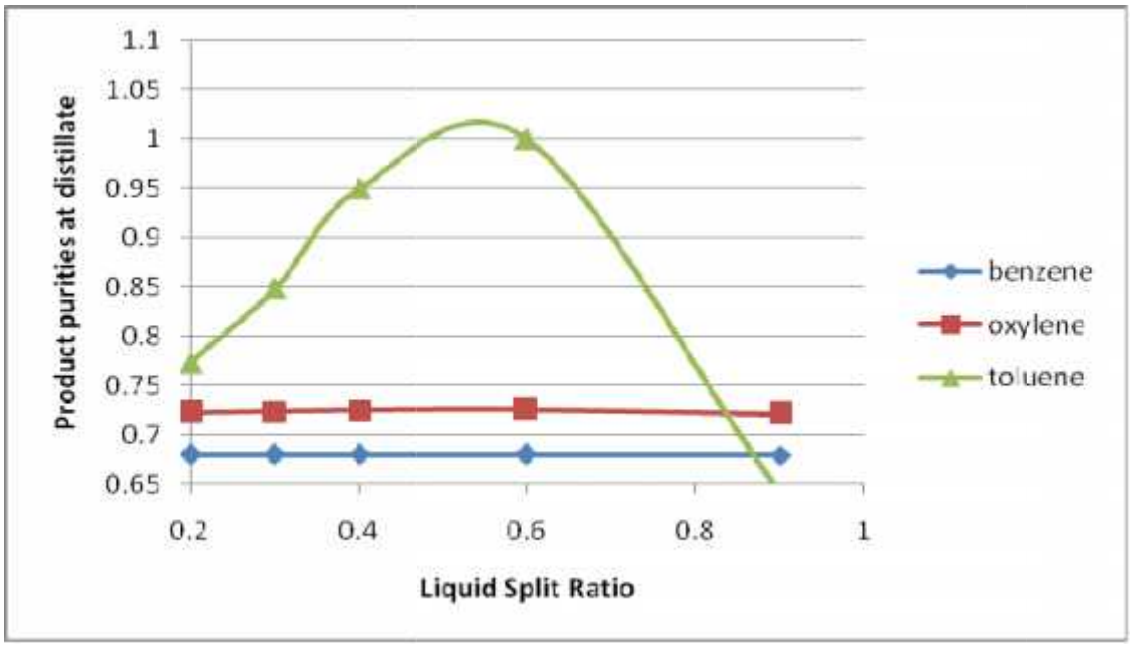


Fig 3.2.5: Graph between Product Purity at distillate v/s Liquid Split Fraction.

EFFECT OF VAPOR SPLIT ON PRODUCT PURITY AT DISTILLATE

The vapour split factor in the dividing wall column decides how much quantity of the vapour will enter in the prefractionator from stripping section. It has been seen that changing the vapor split values from 0.2 to 0.8 , the purities of top and bottom product remain unchanged whereas, the value of side stream purity initially increased with increasing liquid split ratio, achieved a maxima and then started decreasing. The maximum value of Toluene purity (Side Stream) was observed to be at 60% and its value was 99.7% pure.

vapor split ratio	benzene(Top Product)	o-xylene(Bottom Product)	toluene(Side Stream)
0.2	0.67868844	0.72528939	0.95178315

0.4	0.67940059	0.72530188	0.99968688
0.6	0.67940362	0.72526867	0.99703739
0.8	0.67784981	0.72356447	0.76865953

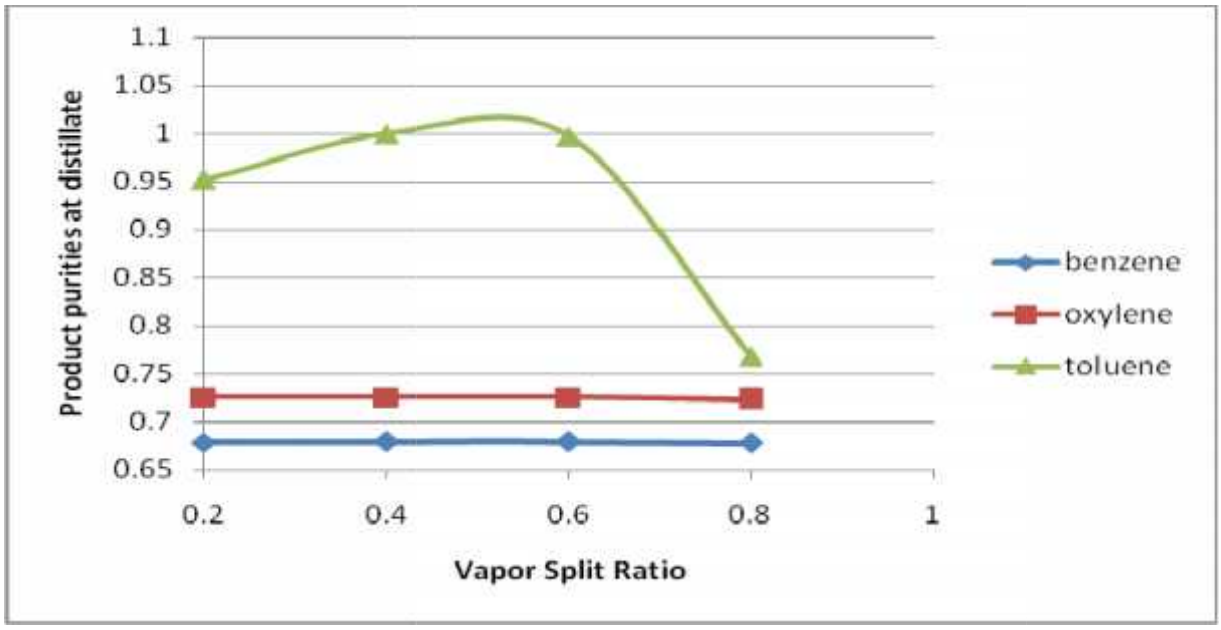


Fig 3.2.6: Graph between Product Purity at distillate v/s Vapor Split Fraction.

EFFECT OF REBOILER DUTY ON PRODUCT PURITY AT DISTILLATE

The reboiler duty was varied from 30 MW to 60 MW. Its effects were seen on Product Purity at distillate. The value of top product (benzene) purity was seen to be decreasing with increasing value of reboiler duty with having a maximum value of 80.8% at 30 MW reboilerduty and a minimum value of 52.3 % at 60 MW reboiler duty. The value of bottom product (o-Xylene) purity was seen observing a reverse trend. It's values were increasing with increasing reboiler duty, with having a maximum value of 95.1% at 60 MW reboiler duty and a minimum value of 30 MW reboiler duty. The values of side stream purity were seemingly unfazed.

REBOILER DUTY(M.W)	BENZENE(Top Product)	o-XYLENE(Bottom	TOLUENE(Side Stream)

		Product)	
30	0.80897258	0.64286142	0.99976595
35	0.74202423	0.67939788	0.99987731
40.54	0.67940499	0.72530247	0.99991408
45	0.63606631	0.76715044	0.99992819
50	0.59357792	0.82026788	0.99993822
55	0.55644201	0.88122272	0.99994532
60	0.52378014	0.95169385	0.99995075

Fig 3.2.7: Graph between Product Purity at distillate v/s Reboiler Duty.

3.3SIMULATION OF SEPARATION OF A TERNARY MIXTURE OF METHANOL GLYCEROL AND WATER

DETAILS OF SIMULATION.

Table 3.3**:** Modelling Details for the separation of ternary mixture of Methanol-Glycerol-Water using dividing wall distillation column.

PARAMETERS AND CONDITIONS			**VALUE**
FEED FLOW RATE			100 Kmols/Hr
FEED COMPOSITION	Methanol	Mol Fraction	0.2
	Glycerol		0.5
	Water		0.3
Number of trays in Prefractionator (B1)			7
Number of trays in Top Section (B2)			10
Number of trays in Bottom Section (B3)			10
Number of trays in Side Draw (B4)			7
Feed tray Position			3^{rd}stage of pre-fractionator
Side Draw Position			6^{th} of main column
Reboiler Duty			1883 kW
Split Ratio	Liquid Split		0.4
	Vapor Split		0.4

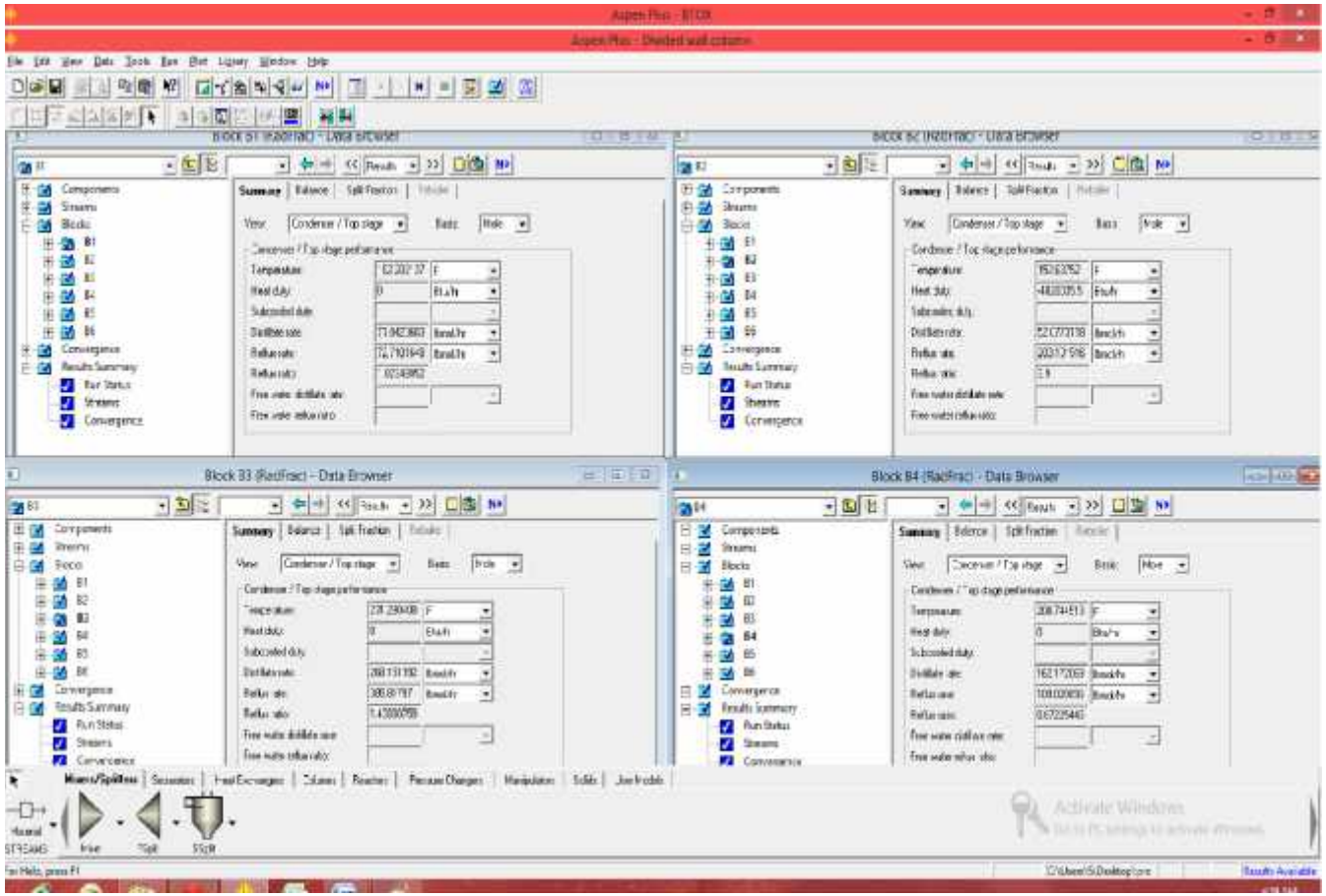


Fig 3.3.1: Blocks Summary for Chapter 3.3.

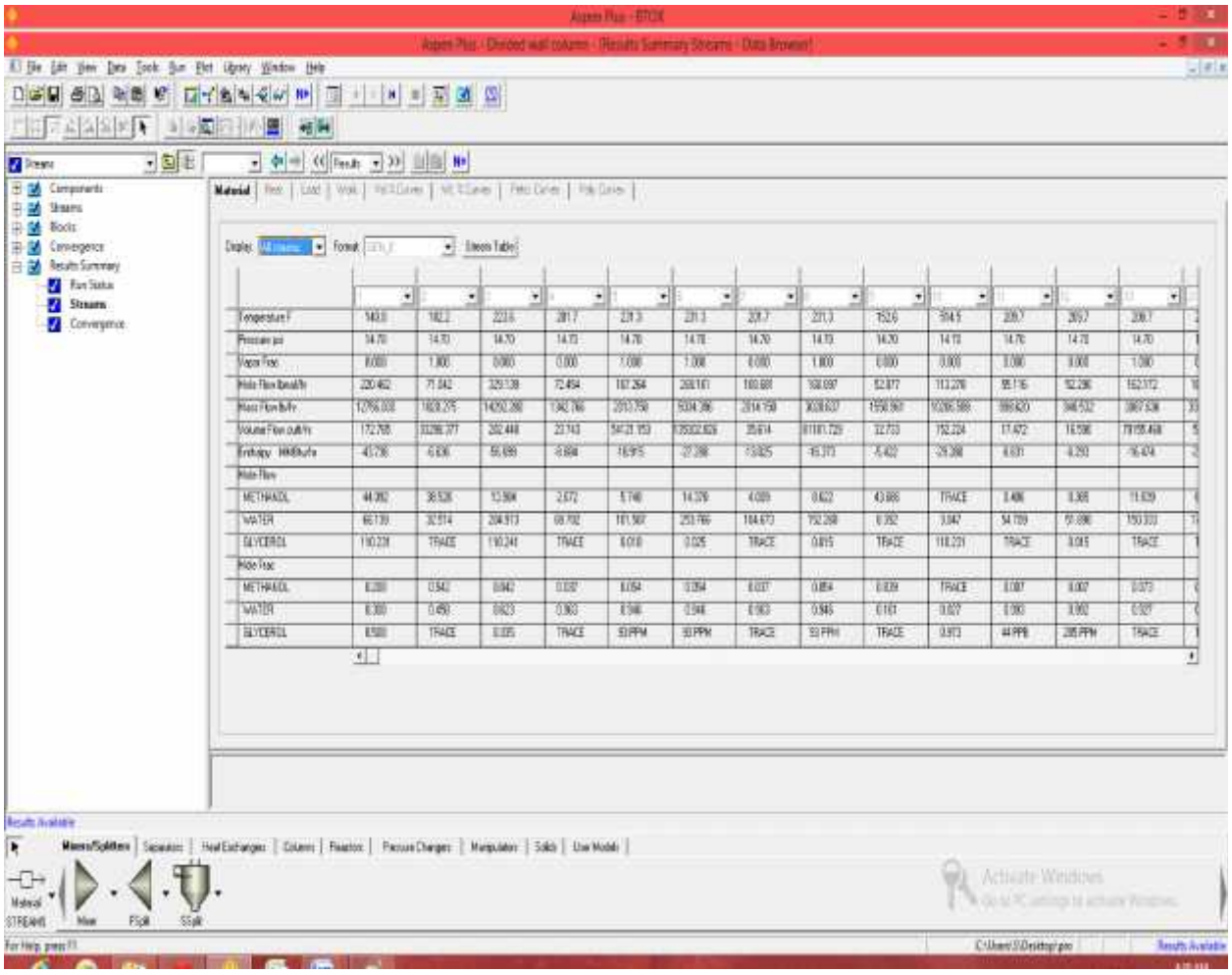


Fig 3.3.2: Results Summary for chapter 3.3.

EFFECT OF REFLUX RATIO ON PRODUCT PURITY AT DISTILLATE

In the dividing wall column, reflux ratio plays an important role.s the reflux ratio is increased, the gradient of operating line for the rectification section moves towards a maximum value of 1. Physically, what this means is that more and more liquid that is rich in the more volatile components are being recycled back into the column.When more overhead liquid product is refluxed in a distillation column the liquid rate in the column increases. Separation then becomes better. The effect of reflux ratio was seen on Product Purity at distillate by varying reflux ratio from 3.5 to 3.9. The top product (Methanol) purity was seen to change from 80.5% to 83.8%, whereas the bottom product (Glycerol) purity decreased with increasing reflux Ratio. It's value changed from 99.2% to 97.3%. The purity of side stream (Water) was seemingly unfazed by changes in reflux ratio.

REFLUX RATIO	PURITY METHANOL(Top Product)	GLYCEROL(Bottom Product)	WATER(Side Stream)
3.5	0.80561795	0.99103407	0.9910987
3.6	0.81397307	0.98637591	0.99151228
3.7	0.82238353	0.98187618	0.99189927
3.8	0.83068241	0.97745747	0.99227147
3.9	0.83886211	0.97310562	0.99263036

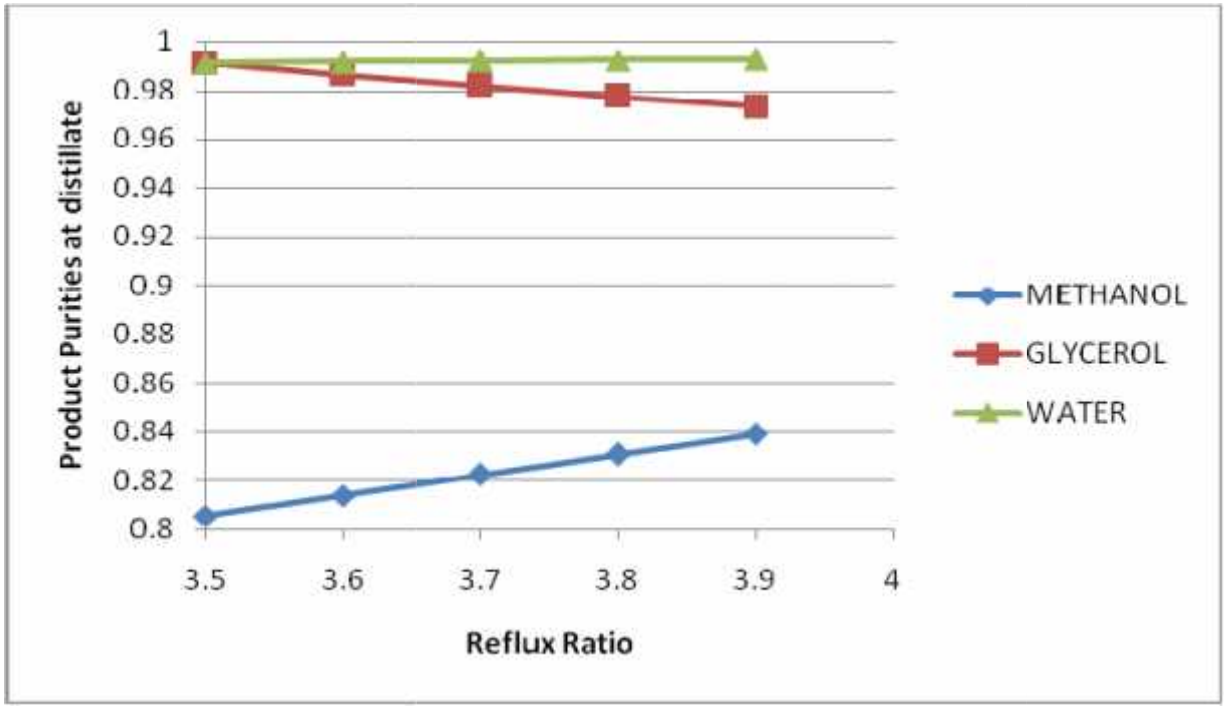


Fig 3.3.3: Graph between Product Purity at distillate v/s Reflux Ratio.

EFFECT OF FEED STAGE ON PRODUCT PURITY AT DISTILLATE

Selection of feed stage is an important factor for Product Purity at distillate. As the feed stage is moved lower down the column, the top composition becomes less rich in the more volatile component while the bottoms contains more of the more volatile component.Generally speaking, if the feed enters in higher tray the light components concentrations in overhead will be increased and in bottom outlet will be decreased. As the feed stage is moved lower down the column, the top composition becomes less rich in the more volatile component while the bottoms contains more of the more volatile component. It was seen that for the particular ternary mixture of Methanol-Glycerol-Water, the Product Purity at distillate didn't change appreciably with changing feed tray position.

FEED POSITION	METHANOL(Top Product)	GLYCEROL(Bottom Product)	WATER(Side Stream)
3	0.83886211	0.97310562	0.99263036
4	0.83686304	0.9730468	0.99056924
5	0.83539385	0.97301463	0.98900755
6	0.83369679	0.97295536	0.98727789

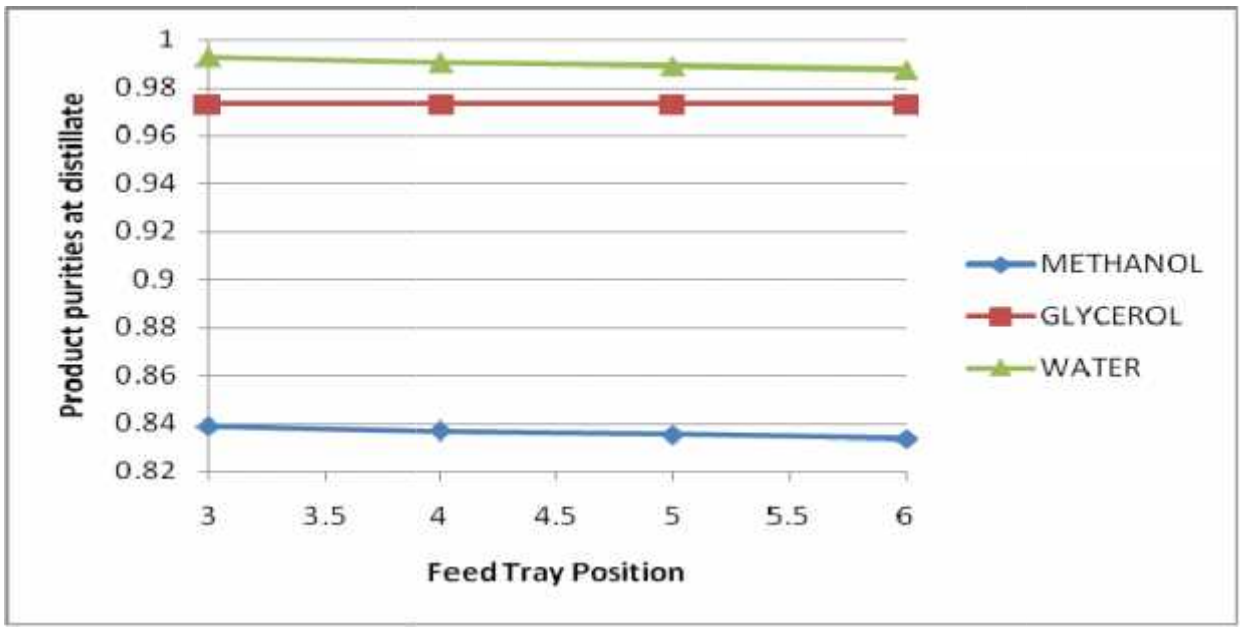


Fig 3.3.4: Graphs between Product Purity at distillate v/s Feed Stage.

EFFECT OF LIQUID SPLIT FRACTION ON PRODUCT PURITY AT DISTILLATE

The liquid split factor in the dividing wall column decides how much quantity of the liquid will enter the prefractionator from the rectifying section. As we are supplying the feed in the prefractionator column, the fraction of liquid to be distributed coming from the rectifying section should be less in comparison with the main column to maintain the liquid hold up in both sections. The liquid split ratio was changed from 30% to 60% and its effects on the Product Purity at distillate were seen. Though the effects were not as pronounced as the ones in the previous cases, the product purities of both Top product and side stream were slightly decreasing from 84.1% to 83.4% and 99.5% to 98.7% respectively.

Liquid split ratio	methanol(Top Product)	glycerol(Bottom Product)	water(Side Stream)
0.3	0.84169546	0.9732641	0.99532581
0.4	0.83886211	0.97310562	0.99263036
0.5	0.83640979	0.97302374	0.99012187
0.6	0.83412708	0.97294435	0.98781901

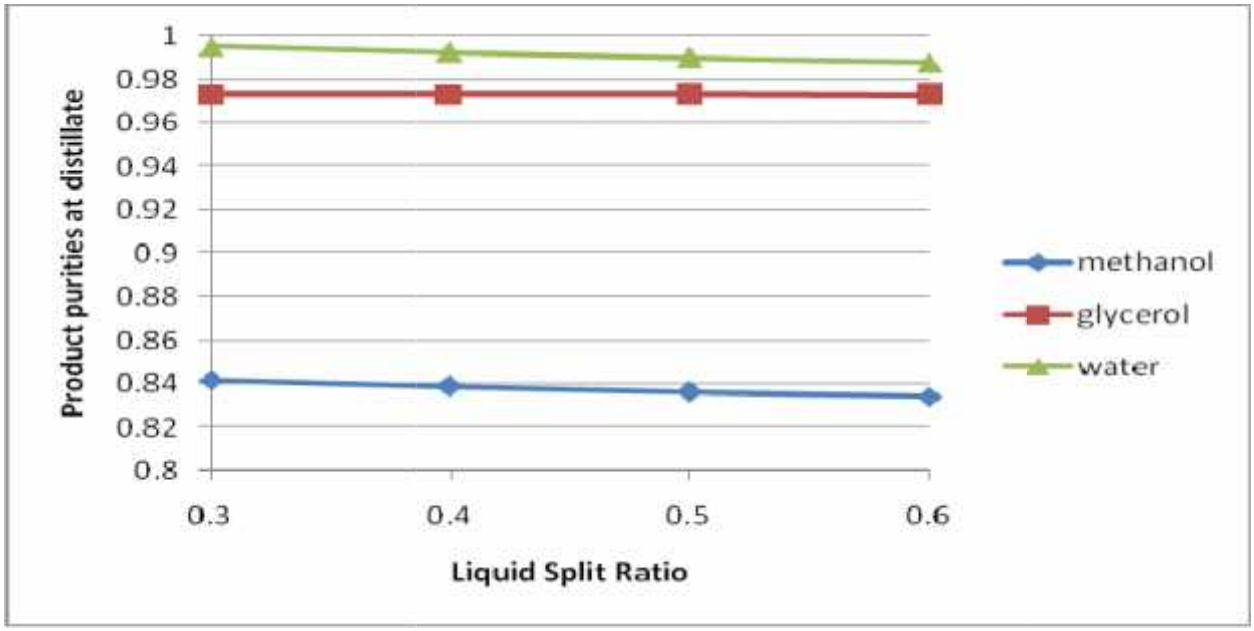


Fig 3.3.5: Graph between Product Purity at distillate v/s Liquid Split Fraction.

EFFECT OF VAPOR SPLIT ON PRODUCT PURITY AT DISTILLATE

The vapor split factor in the dividing wall column decides how much quantity of the vapour will enter in the prefractionator from stripping section. The values of vapor split fraction were changed from 30% to 70% and their effects on the Product Purity at distillate were seen. While the bottom prduct purity did not change significantly, both the top product and side stream purities increased gradually achieved maxima and then stayed constant.

vapor split ratio	methanol(Top Product)	glycerol(Bottom Product)	water(Side Stream)
0.3	0.82596075	0.97262408	0.97965137
0.4	0.83886211	0.97310562	0.99263036
0.5	0.84611211	0.97339913	0.99986962
0.6	0.84625214	0.97341345	0.9999763
0.7	0.84624135	0.97340079	0.99999078

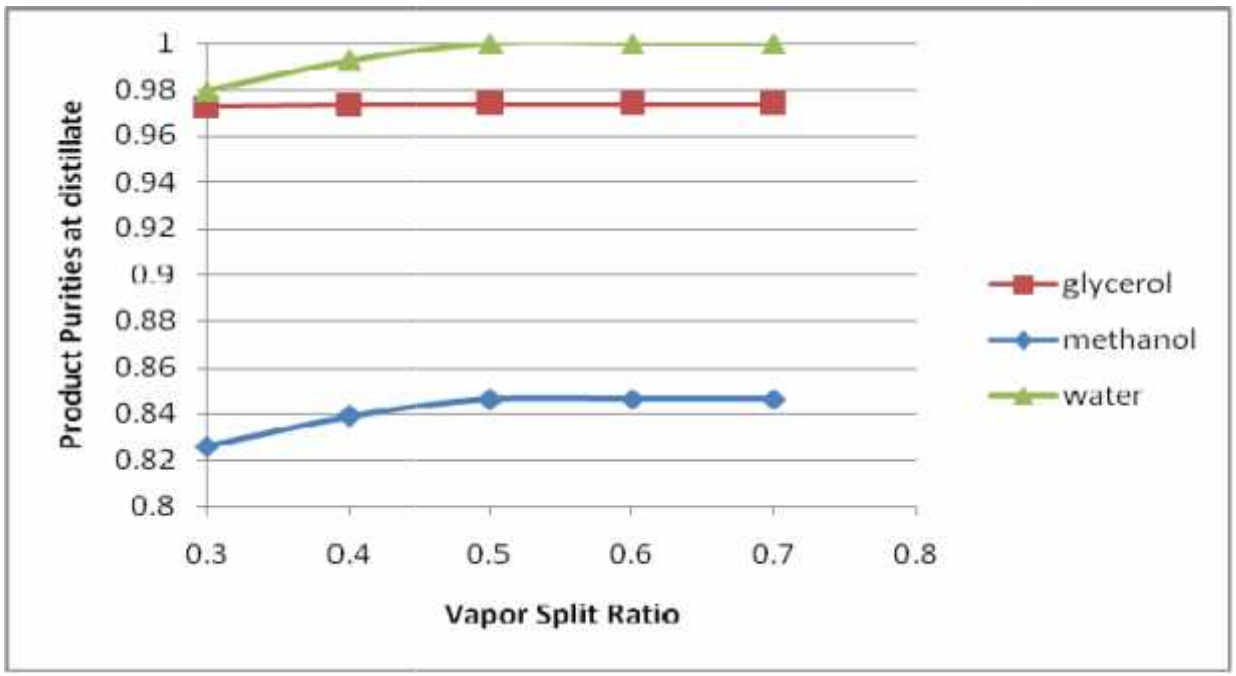


Fig 3.3.6: Graph between Product Purity at distillate v/s Vapor Split Fraction.

EFFECT OF REBOILER DUTY ON PRODUCT PURITY AT DISTILLATE

The reboiler duty of stripping column was varied from 1650 kW to 2000 kW and no marked change was seen regarding the Product Purity at distillate of any of the product i.e, top , bottom and side stream. This remarks that a Dividing Wall Column is equally efficient at lower energy consumptions even.

REBOILER DUTY(M.W)	METHANOL(Top Product)	GLYCEROL(Bottom Product)	WATER(Side Stream)
2	0.83887	0.9731	0.994813555
1.95	0.84027	0.9731	0.993922719
1.883	0.83886	0.9731	0.992622549
1.8	0.83691	0.9731	0.99076329
1.75	0.83555	0.9731	0.989514522
1.7	0.83409	0.9731	0.988130766
1.65	0.83246	0.9731	0.986565511

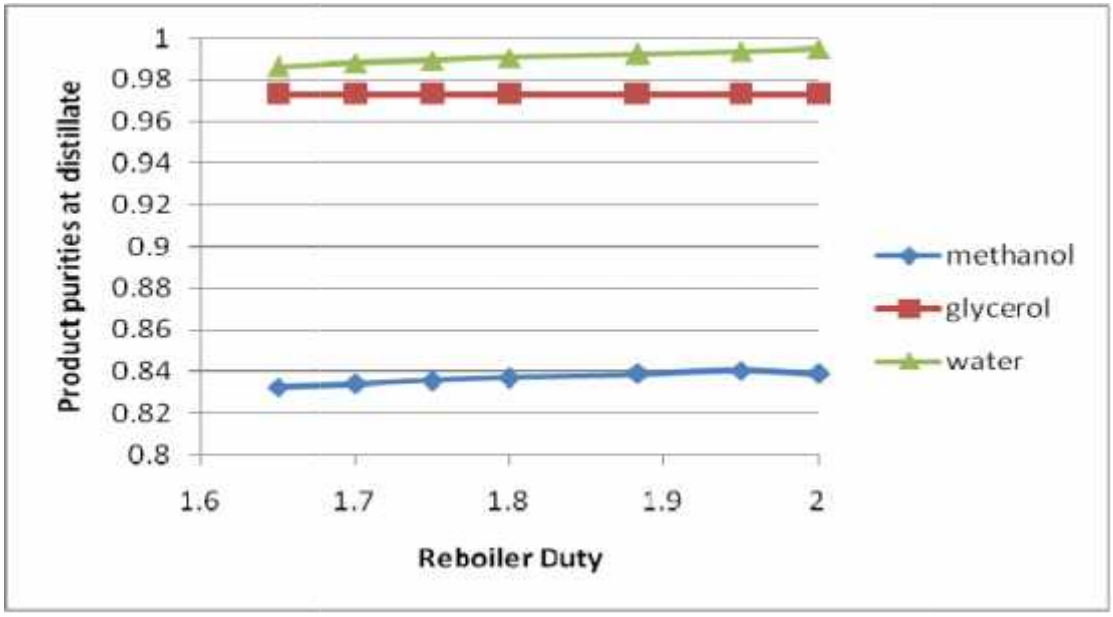


Fig 3.3.7: Graph between Product Purity at distillate v/s Reboiler Duty.

CONCLUSIONS

An Aspen Simulation was developed for a dividing wall column, which has been used toinvestigate the parametric effects of several parameters such as reflux ratio, feed stage, liquid split factor, vapor split factor and reboiler ratio on Product Purity at distillate were observed. It was seen uniformly in all three simulations that increasing the reflux ratio results in the following-

Increase in the top Product Purity at distillate, Decrease in the bottom Product Purity at distillate and no pronounced change in the purity of side stream.

The effect of feed stage on Product Purity at distillate, uniformly in all three simulations was found to be as follows,

Increasing the Feed tray position didn’t have any pronounced effect over the top and bottom product purities. However, the side stream Product Purity at distillate uniformly decreased slightly in all three cases.

The effects of liquid and vapor split fractions on Product Purity at distillate though non-uniform for all the three cases but the general trend was that the top product and side stream purities initially increased upto a certain value, achieved maxima and then started decreasing very gradually. The maxima values are the optimum values of liquid and vapor fraction.

The effect of reboiler duty on product purities was that with increasing reboiler duty, the product purities increased with an odd case or two.

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